



# Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 02:01 PM GMT

PDB ID : 1JRA  
Title : Crystal Structure of Erv2p  
Authors : Gross, E.; Sevier, C.S.; Vala, A.; Kaiser, C.A.; Fass, D.  
Deposited on : 2001-08-13  
Resolution : 2.00 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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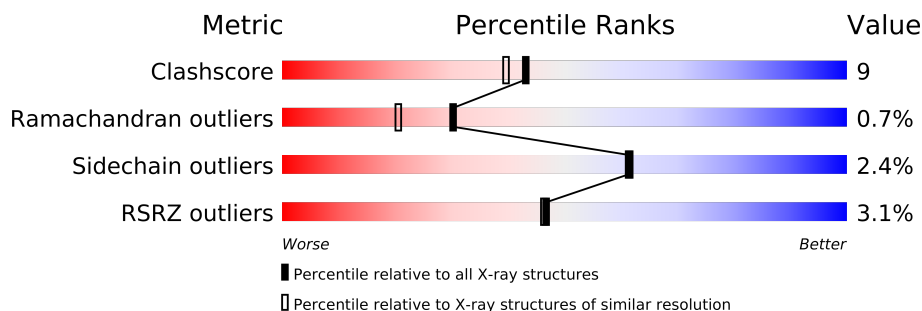
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 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 2.00 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))
Clashscore	79885	6188 (2.00-2.00)
Ramachandran outliers	78287	6102 (2.00-2.00)
Sidechain outliers	78261	6100 (2.00-2.00)
RSRZ outliers	66119	4890 (2.00-2.00)

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. 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	117	
1	B	117	
1	C	117	
1	D	117	

## 2 Entry composition i

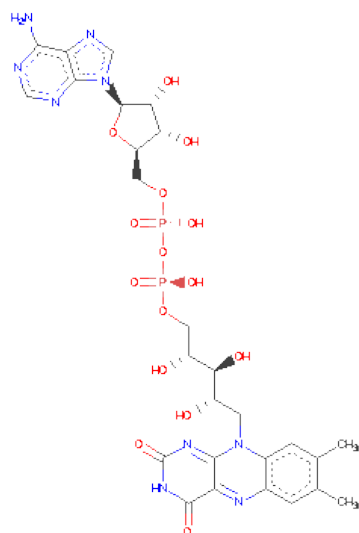
There are 3 unique types of molecules in this entry. The entry contains 3944 atoms, of which 0 are hydrogen and 0 are deuterium.

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 ERV2 PROTEIN, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	106	Total	C	N	O	S	0	0	0
			868	556	143	162	7			
1	B	106	Total	C	N	O	S	0	0	0
			868	556	143	162	7			
1	C	105	Total	C	N	O	S	0	0	0
			862	553	142	160	7			
1	D	103	Total	C	N	O	S	0	0	0
			846	545	140	154	7			

- 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	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	82	Total	O	0	0
			82	82		
3	B	73	Total	O	0	0
			73	73		
3	C	73	Total	O	0	0
			73	73		
3	D	60	Total	O	0	0
			60	60		

### 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.

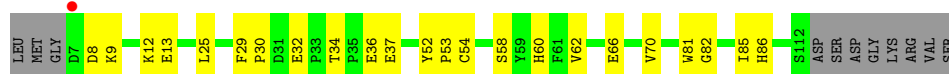
- Molecule 1: ERV2 PROTEIN, MITOCHONDRIAL

Chain A: 



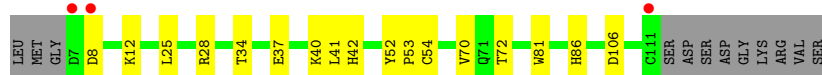
- Molecule 1: ERV2 PROTEIN, MITOCHONDRIAL

Chain B: 



- Molecule 1: ERV2 PROTEIN, MITOCHONDRIAL

Chain C: 



- Molecule 1: ERV2 PROTEIN, MITOCHONDRIAL

Chain D: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	53.63Å 66.81Å 60.38Å 90.00° 91.44° 90.00°	Depositor
Resolution (Å)	20.00 – 2.00 19.88 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.5 (20.00-2.00) 99.8 (19.88-2.00)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.81 (at 2.01Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.196 , 0.233 0.202 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	22.5	Xtriage
Anisotropy	0.064	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 35.5	EDS
Estimated twinning fraction	0.034 for h,-k,-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 28807 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	3944	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.72% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities 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: 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	0.32	0/893	0.53	0/1208
1	B	0.32	0/893	0.53	0/1208
1	C	0.33	0/887	0.53	0/1200
1	D	0.33	0/871	0.53	0/1178
All	All	0.32	0/3544	0.53	0/4794

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 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	868	0	825	20	0
1	B	868	0	825	17	0
1	C	862	0	820	16	0
1	D	846	0	812	17	0
2	A	53	0	29	1	0
2	B	53	0	31	1	0
2	C	53	0	30	1	0
2	D	53	0	31	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	82	0	0	2	0
3	B	73	0	0	1	0
3	C	73	0	0	4	0
3	D	60	0	0	2	0
All	All	3944	0	3403	62	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 9.

All (62) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:53:PRO:HG3	1:D:25:LEU:HA	1.54	0.87
1:A:25:LEU:HA	1:B:53:PRO:HG3	1.67	0.77
1:D:77:ALA:HB3	3:D:393:HOH:O	1.85	0.75
1:C:25:LEU:HA	3:C:374:HOH:O	1.90	0.71
1:B:62:VAL:O	1:B:66:GLU:HG3	1.92	0.69
1:B:34:THR:OG1	1:B:36:GLU:HG2	1.93	0.68
1:C:40:LYS:HE2	1:D:50:GLU:OE2	1.96	0.66
1:A:45:ILE:HD13	1:A:70:VAL:HG21	1.77	0.65
1:D:109:CYS:C	1:D:111:CYS:H	1.99	0.65
1:A:9:LYS:O	1:A:13:GLU:HG3	1.96	0.65
1:D:29:PHE:CD1	1:D:30:PRO:HD2	2.33	0.64
1:D:109:CYS:C	1:D:111:CYS:N	2.55	0.60
1:A:45:ILE:CD1	1:A:70:VAL:HG21	2.31	0.58
1:B:29:PHE:CD1	1:B:30:PRO:HD2	2.37	0.58
1:A:84:HIS:HB3	3:A:354:HOH:O	2.03	0.57
1:B:9:LYS:O	1:B:13:GLU:HG3	2.05	0.57
1:C:70:VAL:HA	1:C:81:TRP:CE2	2.44	0.52
1:C:40:LYS:HG2	3:C:399:HOH:O	2.10	0.52
1:A:28:ARG:HG2	3:A:382:HOH:O	2.10	0.52
1:A:45:ILE:HD13	1:A:70:VAL:CG2	2.39	0.52
1:A:62:VAL:O	1:A:66:GLU:HG3	2.10	0.51
1:B:58:SER:O	1:B:62:VAL:HG23	2.11	0.50
1:C:12:LYS:HA	2:C:337:FAD:H4'	1.95	0.49
1:C:28:ARG:HB3	3:C:374:HOH:O	2.12	0.49
1:A:53:PRO:HG3	1:B:25:LEU:HA	1.93	0.49
1:C:25:LEU:HA	1:D:53:PRO:HG3	1.96	0.48
1:A:8:ASP:OD1	1:A:12:LYS:HE3	2.13	0.48
1:A:25:LEU:CA	1:B:53:PRO:HG3	2.40	0.48
1:B:36:GLU:HG3	1:B:37:GLU:N	2.28	0.48
1:A:41:LEU:O	1:A:45:ILE:HD12	2.14	0.48
1:C:25:LEU:HD23	1:C:25:LEU:C	2.36	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:34:THR:HG1	1:B:36:GLU:HG2	1.80	0.46
1:A:9:LYS:HE3	1:C:106:ASP:OD2	2.16	0.46
1:D:29:PHE:CG	1:D:30:PRO:HD2	2.50	0.46
1:D:41:LEU:HD23	1:D:72:THR:HG22	1.98	0.46
1:D:109:CYS:O	1:D:111:CYS:N	2.49	0.45
1:A:105:GLU:H	1:A:105:GLU:CD	2.20	0.45
1:A:45:ILE:HD13	1:A:70:VAL:CB	2.47	0.45
1:B:70:VAL:HA	1:B:81:TRP:CE2	2.52	0.45
1:B:25:LEU:C	1:B:25:LEU:HD23	2.37	0.44
1:B:8:ASP:O	1:B:12:LYS:HG3	2.18	0.44
1:B:82:GLY:O	1:B:85:ILE:HG22	2.16	0.44
1:C:86:HIS:HD2	1:C:86:HIS:O	2.01	0.44
1:A:25:LEU:C	1:A:25:LEU:HD23	2.38	0.44
1:C:41:LEU:HD23	1:C:72:THR:HG22	2.00	0.44
1:B:52:TYR:HA	1:B:53:PRO:HD3	1.70	0.43
1:C:52:TYR:HA	1:C:53:PRO:HD3	1.76	0.43
1:D:88:LYS:HA	1:D:88:LYS:HZ3	1.82	0.43
1:C:42:HIS:HD2	3:C:357:HOH:O	2.02	0.43
1:B:86:HIS:HE1	2:B:334:FAD:H51A	1.85	0.42
1:D:73:SER:N	3:D:393:HOH:O	2.51	0.42
1:D:30:PRO:HG2	1:D:33:PRO:HB3	2.02	0.41
1:C:53:PRO:HG3	1:D:25:LEU:CA	2.39	0.41
1:D:102:THR:HB	1:D:105:GLU:HB3	2.02	0.41
1:C:34:THR:OG1	1:C:37:GLU:HG3	2.21	0.41
1:B:60:HIS:HE1	3:B:391:HOH:O	2.03	0.41
1:A:86:HIS:HB3	2:A:335:FAD:N6A	2.36	0.41
1:A:52:TYR:HA	1:A:53:PRO:HD3	1.72	0.41
1:A:68:TYR:CZ	1:A:88:LYS:HE2	2.55	0.41
1:D:86:HIS:O	1:D:86:HIS:HD2	2.03	0.41
1:D:52:TYR:HA	1:D:53:PRO:HD3	1.72	0.41
1:A:105:GLU:CD	1:A:105:GLU:N	2.74	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	104/117 (89%)	102 (98%)	1 (1%)	1 (1%)	22	12
1	B	104/117 (89%)	100 (96%)	4 (4%)	0	100	100
1	C	103/117 (88%)	100 (97%)	2 (2%)	1 (1%)	22	12
1	D	101/117 (86%)	94 (93%)	6 (6%)	1 (1%)	22	12
All	All	412/468 (88%)	396 (96%)	13 (3%)	3 (1%)	30	20

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	108	ASP
1	C	8	ASP
1	A	54	CYS

### 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	94/103 (91%)	92 (98%)	2 (2%)	66	67
1	B	94/103 (91%)	92 (98%)	2 (2%)	66	67
1	C	93/103 (90%)	92 (99%)	1 (1%)	84	86
1	D	91/103 (88%)	87 (96%)	4 (4%)	39	32
All	All	372/412 (90%)	363 (98%)	9 (2%)	61	61

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	54	CYS
1	A	85	ILE
1	B	32	GLU
1	B	54	CYS
1	C	54	CYS
1	D	39	GLU
1	D	54	CYS
1	D	88	LYS
1	D	108	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	60	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	335	-	58,58,58	2.11	13 (22%)	85,89,89	4.24	46 (54%)
2	FAD	B	334	-	58,58,58	2.14	15 (25%)	85,89,89	4.00	35 (41%)
2	FAD	C	337	-	58,58,58	2.12	13 (22%)	85,89,89	4.60	44 (51%)
2	FAD	D	336	-	58,58,58	2.12	12 (20%)	85,89,89	4.13	44 (51%)

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	335	-	-	0/34/50/50	0/1/6/6
2	FAD	B	334	-	-	0/34/50/50	0/1/6/6
2	FAD	C	337	-	-	0/34/50/50	0/1/6/6
2	FAD	D	336	-	-	0/34/50/50	0/1/6/6

All (53) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	336	FAD	C9A-N10	7.25	1.49	1.38
2	B	334	FAD	C9A-N10	7.12	1.49	1.38
2	A	335	FAD	C9A-N10	7.07	1.49	1.38
2	C	337	FAD	C9A-N10	6.86	1.49	1.38
2	A	335	FAD	C4A-N3A	5.24	1.43	1.35
2	B	334	FAD	C4A-N3A	5.07	1.43	1.35
2	D	336	FAD	C4A-N3A	4.80	1.42	1.35
2	C	337	FAD	C4A-N3A	4.79	1.42	1.35
2	B	334	FAD	C2A-N3A	4.78	1.41	1.32
2	D	336	FAD	C2A-N3A	4.78	1.41	1.32
2	A	335	FAD	C5X-N5	4.78	1.42	1.35
2	C	337	FAD	C2A-N3A	4.75	1.41	1.32
2	D	336	FAD	C5X-N5	4.64	1.42	1.35
2	C	337	FAD	C1'-N10	-4.57	1.43	1.48
2	B	334	FAD	C5X-N5	4.54	1.42	1.35
2	D	336	FAD	C1'-N10	-4.39	1.43	1.48
2	A	335	FAD	C2A-N3A	4.34	1.40	1.32
2	C	337	FAD	C5X-N5	4.33	1.42	1.35
2	A	335	FAD	C1'-N10	-4.28	1.43	1.48
2	B	334	FAD	C1'-N10	-4.18	1.43	1.48
2	B	334	FAD	C8A-N9A	4.01	1.42	1.36
2	C	337	FAD	C4X-N5	3.89	1.44	1.36
2	A	335	FAD	C8A-N9A	3.89	1.42	1.36
2	D	336	FAD	C8A-N9A	3.82	1.42	1.36
2	B	334	FAD	C4X-N5	3.71	1.43	1.36
2	C	337	FAD	C8A-N9A	3.70	1.42	1.36
2	D	336	FAD	C5A-C4A	-3.66	1.32	1.40
2	C	337	FAD	C5A-C4A	-3.64	1.32	1.40
2	A	335	FAD	C4X-N5	3.55	1.43	1.36
2	D	336	FAD	C4X-N5	3.52	1.43	1.36
2	B	334	FAD	C5A-C4A	-3.44	1.32	1.40
2	D	336	FAD	C9A-C5X	3.21	1.49	1.42
2	A	335	FAD	C5A-C4A	-3.20	1.33	1.40
2	C	337	FAD	C9A-C5X	3.17	1.49	1.42
2	A	335	FAD	C4-N3	3.13	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	334	FAD	C9A-C5X	3.08	1.48	1.42
2	B	334	FAD	C4-N3	3.06	1.42	1.37
2	A	335	FAD	C9A-C5X	2.97	1.48	1.42
2	C	337	FAD	C4-N3	2.91	1.42	1.37
2	D	336	FAD	C4-N3	2.83	1.42	1.37
2	B	334	FAD	C5'-C4'	-2.73	1.47	1.51
2	D	336	FAD	C5'-C4'	-2.64	1.47	1.51
2	A	335	FAD	C5'-C4'	-2.60	1.47	1.51
2	A	335	FAD	C2B-C3B	-2.49	1.46	1.53
2	C	337	FAD	C5'-C4'	-2.45	1.47	1.51
2	D	336	FAD	C2B-C3B	-2.39	1.46	1.53
2	B	334	FAD	C2B-C3B	-2.35	1.46	1.53
2	C	337	FAD	C2B-C3B	-2.30	1.47	1.53
2	C	337	FAD	C8A-N7A	-2.20	1.30	1.34
2	A	335	FAD	C8A-N7A	-2.16	1.30	1.34
2	B	334	FAD	C4A-N9A	2.08	1.40	1.37
2	B	334	FAD	O4B-C1B	2.03	1.44	1.41
2	B	334	FAD	C8A-N7A	-2.01	1.30	1.34

All (169) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	337	FAD	C8A-N9A-C4A	-17.01	93.91	106.90
2	C	337	FAD	N3A-C2A-N1A	-16.00	115.33	128.71
2	D	336	FAD	N3A-C2A-N1A	-14.93	116.23	128.71
2	A	335	FAD	C8A-N9A-C4A	-14.15	96.10	106.90
2	B	334	FAD	C8A-N9A-C4A	-13.55	96.56	106.90
2	C	337	FAD	C4X-C10-N10	-13.33	113.86	120.51
2	D	336	FAD	C4X-C10-N10	-13.32	113.86	120.51
2	D	336	FAD	C8A-N9A-C4A	-13.02	96.96	106.90
2	C	337	FAD	C2-N1-C10	12.97	128.05	114.98
2	A	335	FAD	N3A-C2A-N1A	-12.56	118.21	128.71
2	B	334	FAD	N3A-C2A-N1A	-12.36	118.38	128.71
2	A	335	FAD	C2-N1-C10	12.31	127.38	114.98
2	A	335	FAD	C4X-C10-N10	-11.55	114.75	120.51
2	B	334	FAD	C2-N1-C10	11.47	126.54	114.98
2	B	334	FAD	C4X-C10-N10	-11.25	114.89	120.51
2	B	334	FAD	C4X-N5-C5X	10.95	128.99	116.69
2	C	337	FAD	C9A-N10-C10	10.89	132.45	121.77
2	D	336	FAD	C2-N1-C10	10.32	125.38	114.98
2	A	335	FAD	C4X-N5-C5X	9.92	127.84	116.69
2	A	335	FAD	C9A-N10-C10	9.92	131.50	121.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	334	FAD	C9A-N10-C10	9.60	131.19	121.77
2	C	337	FAD	C4X-N5-C5X	9.26	127.10	116.69
2	D	336	FAD	C9A-N10-C10	9.23	130.82	121.77
2	C	337	FAD	O4B-C1B-N9A	7.94	115.82	108.44
2	D	336	FAD	C4X-N5-C5X	7.23	124.81	116.69
2	A	335	FAD	C2'-C1'-N10	7.14	121.92	112.45
2	A	335	FAD	O4B-C1B-N9A	6.76	114.72	108.44
2	C	337	FAD	C5A-C4A-N9A	6.57	116.66	107.16
2	C	337	FAD	C4'-C3'-C2'	6.48	127.89	113.25
2	D	336	FAD	C8M-C8-C9	-6.43	104.87	120.38
2	D	336	FAD	C8M-C8-C7	6.41	135.55	120.74
2	B	334	FAD	C2'-C1'-N10	6.39	120.93	112.45
2	A	335	FAD	C5'-C4'-C3'	6.38	124.11	112.06
2	C	337	FAD	C5X-C9A-N10	-6.29	110.61	116.80
2	D	336	FAD	O4B-C4B-C5B	-5.93	88.19	109.36
2	D	336	FAD	C5X-C9A-N10	-5.84	111.06	116.80
2	A	335	FAD	C9-C9A-N10	5.82	134.12	121.59
2	D	336	FAD	C2'-C1'-N10	5.74	120.07	112.45
2	B	334	FAD	O4B-C4B-C5B	-5.74	88.87	109.36
2	A	335	FAD	C5B-C4B-C3B	5.73	138.18	115.21
2	C	337	FAD	C9-C9A-N10	5.73	133.93	121.59
2	C	337	FAD	C2'-C1'-N10	5.72	120.04	112.45
2	D	336	FAD	C9-C9A-N10	5.52	133.47	121.59
2	A	335	FAD	C1'-C2'-C3'	5.43	125.35	109.82
2	A	335	FAD	C4X-C10-N1	-5.37	117.37	122.73
2	A	335	FAD	C5X-C9A-N10	-5.27	111.61	116.80
2	D	336	FAD	C1B-N9A-C4A	5.24	135.69	126.64
2	D	336	FAD	O4B-C1B-N9A	5.22	113.30	108.44
2	C	337	FAD	C5B-C4B-C3B	5.21	136.09	115.21
2	B	334	FAD	C8M-C8-C9	-5.19	107.85	120.38
2	C	337	FAD	C1'-N10-C10	-5.19	111.80	119.17
2	D	336	FAD	C2B-C1B-N9A	5.18	126.56	113.27
2	B	334	FAD	C9-C9A-N10	5.03	132.43	121.59
2	B	334	FAD	C1'-N10-C10	-4.91	112.19	119.17
2	A	335	FAD	O3B-C3B-C4B	-4.91	96.61	111.08
2	B	334	FAD	C8M-C8-C7	4.90	132.06	120.74
2	B	334	FAD	C5X-C9A-N10	-4.89	111.99	116.80
2	B	334	FAD	O3P-PA-O5B	-4.83	81.80	103.41
2	C	337	FAD	N3-C2-N1	-4.81	110.96	121.19
2	C	337	FAD	O4B-C4B-C5B	-4.77	92.32	109.36
2	B	334	FAD	O5B-PA-O1A	4.74	127.95	109.37
2	D	336	FAD	O3B-C3B-C2B	4.61	126.82	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	335	FAD	C4A-C5A-N7A	4.56	113.43	109.52
2	D	336	FAD	C5B-C4B-C3B	4.53	133.38	115.21
2	A	335	FAD	N1-C10-N10	4.53	127.88	115.97
2	B	334	FAD	N3-C2-N1	-4.52	111.59	121.19
2	A	335	FAD	C8A-N9A-C1B	4.46	135.17	126.38
2	B	334	FAD	C9A-C5X-N5	-4.42	115.59	122.37
2	C	337	FAD	O5B-PA-O1A	4.40	126.59	109.37
2	A	335	FAD	N3-C2-N1	-4.37	111.91	121.19
2	D	336	FAD	N1-C10-N10	4.35	127.40	115.97
2	C	337	FAD	O5'-P-O1P	-4.34	92.38	109.37
2	A	335	FAD	C1'-N10-C9A	-4.32	114.67	118.87
2	C	337	FAD	N1-C10-N10	4.26	127.18	115.97
2	D	336	FAD	C1'-N10-C10	-4.12	113.31	119.17
2	A	335	FAD	O2A-PA-O1A	4.07	134.92	112.21
2	B	334	FAD	C2B-C1B-N9A	4.01	123.55	113.27
2	D	336	FAD	C4X-C10-N1	-4.00	118.74	122.73
2	D	336	FAD	C1'-C2'-C3'	3.97	121.16	109.82
2	B	334	FAD	N1-C10-N10	3.92	126.28	115.97
2	A	335	FAD	O5B-C5B-C4B	-3.92	94.55	108.94
2	B	334	FAD	C4X-C10-N1	-3.91	118.82	122.73
2	A	335	FAD	C1'-N10-C10	-3.90	113.64	119.17
2	A	335	FAD	C9A-C5X-N5	-3.89	116.41	122.37
2	A	335	FAD	O3P-PA-O5B	-3.88	86.06	103.41
2	C	337	FAD	C8M-C8-C7	3.87	129.69	120.74
2	C	337	FAD	O2'-C2'-C3'	3.84	118.61	109.05
2	B	334	FAD	C8A-N9A-C1B	3.83	133.93	126.38
2	C	337	FAD	C4X-C10-N1	-3.79	118.94	122.73
2	D	336	FAD	N3-C2-N1	-3.77	113.18	121.19
2	B	334	FAD	C5B-C4B-C3B	3.76	130.28	115.21
2	C	337	FAD	C2A-N1A-C6A	3.76	125.55	118.77
2	D	336	FAD	P-O3P-PA	3.75	142.69	131.68
2	D	336	FAD	O2P-P-O3P	3.75	122.93	105.14
2	C	337	FAD	C2B-C1B-N9A	3.72	122.82	113.27
2	A	335	FAD	C8M-C8-C7	3.70	129.28	120.74
2	D	336	FAD	O2A-PA-O1A	3.67	132.71	112.21
2	B	334	FAD	O4'-C4'-C3'	3.64	118.10	109.05
2	C	337	FAD	C8A-N9A-C1B	3.60	133.48	126.38
2	B	334	FAD	C5A-C4A-N9A	3.55	112.29	107.16
2	B	334	FAD	C5'-C4'-C3'	3.54	118.74	112.06
2	C	337	FAD	PA-O5B-C5B	3.49	147.15	122.03
2	C	337	FAD	C8M-C8-C9	-3.45	112.06	120.38
2	C	337	FAD	C1B-N9A-C4A	3.44	132.59	126.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	337	FAD	C1'-N10-C9A	-3.40	115.57	118.87
2	A	335	FAD	C4B-O4B-C1B	-3.36	106.09	109.75
2	B	334	FAD	C1'-C2'-C3'	3.36	119.42	109.82
2	C	337	FAD	C9A-C5X-N5	-3.35	117.23	122.37
2	A	335	FAD	C8M-C8-C9	-3.35	112.30	120.38
2	B	334	FAD	C5A-C6A-N6A	-3.34	113.17	120.72
2	B	334	FAD	C6-C5X-N5	3.32	122.85	118.97
2	C	337	FAD	N3A-C4A-N9A	-3.30	119.47	125.43
2	D	336	FAD	O3P-PA-O5B	-3.30	88.63	103.41
2	B	334	FAD	C4B-O4B-C1B	-3.28	106.18	109.75
2	B	334	FAD	O2A-PA-O1A	3.19	130.05	112.21
2	D	336	FAD	C1'-N10-C9A	-3.11	115.84	118.87
2	D	336	FAD	C5A-C4A-N9A	3.11	111.66	107.16
2	A	335	FAD	C9-C9A-C5X	-3.07	114.27	119.38
2	B	334	FAD	C10-C4X-N5	-3.01	116.80	120.45
2	C	337	FAD	C4A-C5A-N7A	-3.01	106.94	109.52
2	D	336	FAD	N6A-C6A-N1A	2.97	125.19	119.36
2	D	336	FAD	C4'-C3'-C2'	2.96	119.93	113.25
2	D	336	FAD	O5B-PA-O1A	2.90	120.75	109.37
2	D	336	FAD	C4A-C5A-N7A	2.90	112.01	109.52
2	B	334	FAD	C4'-C3'-C2'	2.87	119.74	113.25
2	A	335	FAD	O4'-C4'-C5'	-2.83	104.32	110.12
2	A	335	FAD	O4B-C4B-C5B	-2.80	99.35	109.36
2	D	336	FAD	C2A-N1A-C6A	2.80	123.83	118.77
2	C	337	FAD	C5'-C4'-C3'	2.78	117.31	112.06
2	C	337	FAD	O4'-C4'-C5'	-2.75	104.46	110.12
2	A	335	FAD	N7A-C8A-N9A	2.75	122.15	114.36
2	B	334	FAD	C1'-N10-C9A	-2.75	116.20	118.87
2	C	337	FAD	C4B-O4B-C1B	-2.73	106.79	109.75
2	A	335	FAD	C6-C5X-C9A	2.71	122.78	119.02
2	C	337	FAD	O3P-PA-O5B	-2.65	91.55	103.41
2	A	335	FAD	C5A-C4A-N9A	2.61	110.94	107.16
2	D	336	FAD	C7M-C7-C6	-2.61	114.08	120.38
2	D	336	FAD	PA-O5B-C5B	2.60	140.75	122.03
2	A	335	FAD	O5B-PA-O1A	2.58	119.49	109.37
2	A	335	FAD	O4'-C4'-C3'	2.55	115.40	109.05
2	A	335	FAD	C8-C9-C9A	2.52	124.89	119.81
2	A	335	FAD	O2P-P-O3P	2.51	117.05	105.14
2	D	336	FAD	C9A-C5X-N5	-2.50	118.53	122.37
2	A	335	FAD	C10-C4X-N5	-2.50	117.42	120.45
2	C	337	FAD	C9-C9A-C5X	-2.48	115.24	119.38
2	C	337	FAD	O5B-C5B-C4B	-2.42	100.06	108.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	336	FAD	O2A-PA-O3P	-2.42	93.67	105.14
2	D	336	FAD	C9-C9A-C5X	-2.41	115.36	119.38
2	A	335	FAD	C2B-C1B-N9A	2.41	119.44	113.27
2	C	337	FAD	P-O3P-PA	2.34	138.54	131.68
2	D	336	FAD	C5'-C4'-C3'	2.34	116.47	112.06
2	B	334	FAD	C9-C9A-C5X	-2.34	115.48	119.38
2	D	336	FAD	C5A-C6A-N6A	-2.32	115.47	120.72
2	A	335	FAD	O2'-C2'-C3'	-2.31	103.29	109.05
2	C	337	FAD	C8-C9-C9A	2.31	124.47	119.81
2	C	337	FAD	O2A-PA-O1A	2.27	124.86	112.21
2	D	336	FAD	O4'-C4'-C3'	2.26	114.67	109.05
2	A	335	FAD	C5A-C6A-N6A	-2.24	115.64	120.72
2	B	334	FAD	N6A-C6A-N1A	2.21	123.69	119.36
2	D	336	FAD	O2B-C2B-C1B	-2.19	104.61	111.23
2	D	336	FAD	C6-C5X-C9A	2.16	122.01	119.02
2	D	336	FAD	O5B-C5B-C4B	-2.16	101.01	108.94
2	C	337	FAD	N6A-C6A-N1A	2.11	123.51	119.36
2	A	335	FAD	C2A-N1A-C6A	2.07	122.51	118.77
2	C	337	FAD	C1'-C2'-C3'	2.06	115.70	109.82
2	A	335	FAD	C8A-N7A-C5A	-2.05	97.21	103.58
2	A	335	FAD	C7M-C7-C6	-2.05	115.44	120.38
2	A	335	FAD	PA-O5B-C5B	2.04	136.73	122.03
2	C	337	FAD	O3B-C3B-C2B	2.00	118.36	111.83

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, 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	106/117 (90%)	-0.03	3 (2%) 50 50	13, 21, 35, 48	0
1	B	106/117 (90%)	-0.05	1 (0%) 81 82	12, 21, 35, 47	0
1	C	105/117 (89%)	-0.16	3 (2%) 49 49	10, 18, 35, 51	0
1	D	103/117 (88%)	0.31	6 (5%) 22 22	13, 24, 43, 58	0
All	All	420/468 (89%)	0.01	13 (3%) 47 46	10, 21, 38, 58	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	110	GLY	4.7
1	D	111	CYS	4.5
1	D	109	CYS	3.4
1	B	7	ASP	3.3
1	C	7	ASP	3.2
1	A	112	SER	2.8
1	A	7	ASP	2.7
1	D	105	GLU	2.7
1	D	96	ASP	2.6
1	D	102	THR	2.4
1	C	111	CYS	2.2
1	A	97	ILE	2.2
1	C	8	ASP	2.1

### 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, 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	FAD	D	336	53/53	0.11	-0.85	16,21,25,28	0
2	FAD	C	337	53/53	0.09	-0.92	14,17,21,23	0
2	FAD	A	335	53/53	0.08	-1.27	14,18,22,25	0
2	FAD	B	334	53/53	0.08	-1.32	12,17,20,22	0

### 6.5 Other polymers

There are no such residues in this entry.