



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 09:25 PM GMT

PDB ID : 2OOS
Title : Crystal structure of plasmodium falciparum enoyl ACP reductase with tri-closan reductase
Authors : Tsai, H.
Deposited on : 2007-01-26
Resolution : 2.10 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>

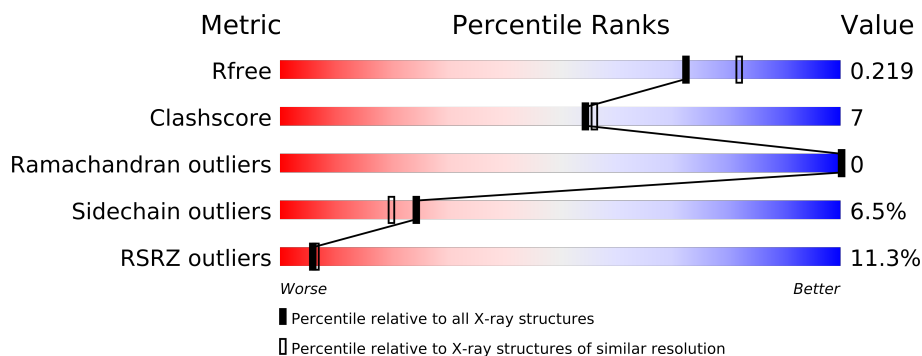
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.10 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}	66092	3012 (2.10-2.10)
Clashscore	79885	3649 (2.10-2.10)
Ramachandran outliers	78287	3610 (2.10-2.10)
Sidechain outliers	78261	3611 (2.10-2.10)
RSRZ outliers	66119	3013 (2.10-2.10)

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	338	
1	B	338	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4805 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 Enoyl-acyl carrier reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	286	Total	C	N	O	S	0	0	0
			2259	1439	379	430	11			
1	B	283	Total	C	N	O	S	0	0	0
			2233	1423	375	424	11			

There are 16 discrepancies between the modelled and reference sequences:

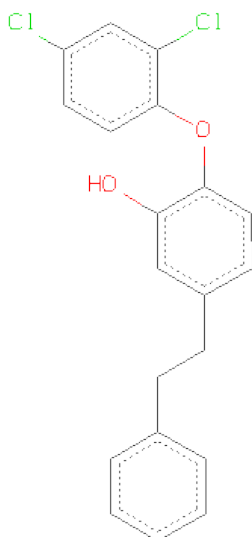
Chain	Residue	Modelled	Actual	Comment	Reference
A	88	MET	-	CLONING ARTIFACT	UNP Q9BH77
A	89	VAL	-	CLONING ARTIFACT	UNP Q9BH77
A	90	HIS	-	EXPRESSION TAG	UNP Q9BH77
A	91	HIS	-	EXPRESSION TAG	UNP Q9BH77
A	92	HIS	-	EXPRESSION TAG	UNP Q9BH77
A	93	HIS	-	EXPRESSION TAG	UNP Q9BH77
A	94	HIS	-	EXPRESSION TAG	UNP Q9BH77
A	95	HIS	-	EXPRESSION TAG	UNP Q9BH77
B	88	MET	-	CLONING ARTIFACT	UNP Q9BH77
B	89	VAL	-	CLONING ARTIFACT	UNP Q9BH77
B	90	HIS	-	EXPRESSION TAG	UNP Q9BH77
B	91	HIS	-	EXPRESSION TAG	UNP Q9BH77
B	92	HIS	-	EXPRESSION TAG	UNP Q9BH77
B	93	HIS	-	EXPRESSION TAG	UNP Q9BH77
B	94	HIS	-	EXPRESSION TAG	UNP Q9BH77
B	95	HIS	-	EXPRESSION TAG	UNP Q9BH77

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: C₂₁H₂₇N₇O₁₄P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 3 is 2-(2,4-DICHLOROPHENOXY)-5-(2-PHENYLETHYL)PHENOL (three-letter code: JPJ) (formula: C₂₀H₁₆Cl₂O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	Cl	O	0	0
			24	20	2	2		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	Cl	O	0	0
			24	20	2	2		

- Molecule 4 is water.

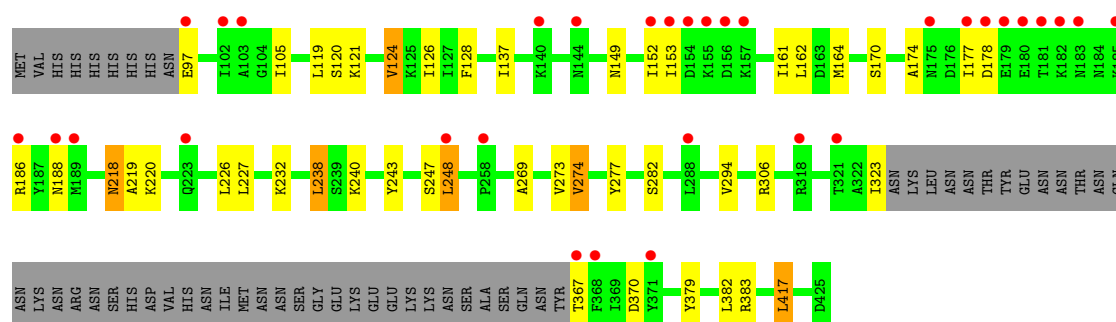
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	86	Total	O	0	0
			86	86		
4	B	91	Total	O	0	0
			91	91		

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.

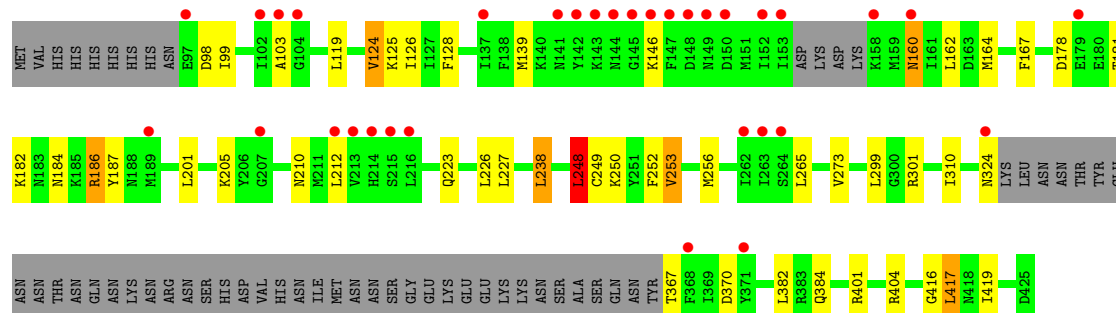
- Molecule 1: Enoyl-acyl carrier reductase

Chain A: 



- Molecule 1: Enoyl-acyl carrier reductase

Chain B: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	131.22Å 131.22Å 83.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	92.85 – 2.10 28.99 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.7 (92.85-2.10) 99.8 (28.99-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.94 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.192 , 0.227 0.185 , 0.219	Depositor DCC
R_{free} test set	2160 reflections (5.31%)	DCC
Wilson B-factor (Å ²)	38.9	Xtriage
Anisotropy	0.189	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 42.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 42847 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	4805	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.53% 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: JPJ, NAD

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	0.85	0/2300	0.85	6/3101 (0.2%)
1	B	0.82	0/2273	0.83	5/3065 (0.2%)
All	All	0.84	0/4573	0.84	11/6166 (0.2%)

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	238	LEU	CA-CB-CG	-8.23	96.38	115.30
1	B	238	LEU	CA-CB-CG	-7.72	97.54	115.30
1	A	248	LEU	CB-CG-CD2	7.12	123.11	111.00
1	A	273	VAL	CG1-CB-CG2	6.34	121.05	110.90
1	B	248	LEU	CA-CB-CG	6.05	129.22	115.30
1	A	417	LEU	CB-CG-CD2	5.71	120.71	111.00
1	A	306	ARG	NE-CZ-NH2	-5.59	117.50	120.30
1	A	248	LEU	CA-CB-CG	5.57	128.12	115.30
1	B	404	ARG	NE-CZ-NH1	5.22	122.91	120.30
1	B	417	LEU	CB-CG-CD2	5.22	119.87	111.00
1	B	238	LEU	CB-CG-CD1	5.11	119.69	111.00

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	2259	0	2269	30	0
1	B	2233	0	2240	36	0
2	A	44	0	26	0	0
2	B	44	0	26	0	0
3	A	24	0	16	2	0
3	B	24	0	16	0	0
4	A	86	0	0	3	0
4	B	91	0	0	2	0
All	All	4805	0	4593	63	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 7.

All (63) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:139:MET:SD	1:B:164:MET:HE2	2.11	0.90
1:B:367:THR:O	1:B:367:THR:HG22	1.73	0.88
1:B:223:GLN:NE2	1:B:324:ASN:HB2	1.90	0.85
1:B:126:ILE:HG21	1:B:128:PHE:HE1	1.45	0.81
1:B:223:GLN:HE21	1:B:324:ASN:H	1.29	0.79
1:B:367:THR:O	1:B:367:THR:CG2	2.35	0.74
1:A:170:SER:HB3	1:A:240:LYS:HD2	1.71	0.73
1:A:277:TYR:HB3	4:A:607:HOH:O	1.90	0.70
1:A:383:ARG:HD3	1:B:301:ARG:HH11	1.56	0.70
1:B:249:CYS:O	1:B:253:VAL:HB	1.97	0.65
1:A:174:ALA:O	1:A:177:ILE:HG12	1.96	0.64
1:B:367:THR:HG23	1:B:370:ASP:HB2	1.79	0.64
1:A:170:SER:HB3	1:A:240:LYS:CD	2.28	0.64
1:B:126:ILE:CG2	1:B:128:PHE:HE1	2.09	0.64
1:B:273:VAL:HG23	4:B:618:HOH:O	1.98	0.63
1:A:220:LYS:HE3	1:A:232:LYS:HE2	1.81	0.62
1:A:218:ASN:HD22	1:A:219:ALA:H	1.44	0.62
1:A:383:ARG:HD3	1:B:301:ARG:NH1	2.15	0.62
1:B:126:ILE:CG2	1:B:128:PHE:CE1	2.83	0.62
1:A:379:TYR:HA	1:B:301:ARG:HH22	1.66	0.61
1:B:184:ASN:ND2	1:B:186:ARG:H	1.97	0.61
1:B:126:ILE:HG21	1:B:128:PHE:CE1	2.34	0.60
1:B:119:LEU:O	1:B:124:VAL:HG13	2.01	0.60
1:A:149:ASN:O	1:A:152:ILE:HG12	2.01	0.59
1:B:99:ILE:HD13	1:B:125:LYS:HB2	1.84	0.59

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:178:ASP:OD1	1:B:181:THR:HG23	2.03	0.59
1:A:170:SER:CB	1:A:240:LYS:HE2	2.32	0.59
1:B:367:THR:CG2	1:B:370:ASP:HB2	2.34	0.58
1:A:119:LEU:O	1:A:124:VAL:HG13	2.04	0.58
1:A:294:VAL:HG11	4:A:605:HOH:O	2.05	0.56
1:A:269:ALA:HB2	1:A:274:VAL:HG13	1.88	0.55
1:B:253:VAL:HG21	1:B:299:LEU:HD22	1.89	0.55
1:A:170:SER:HB3	1:A:240:LYS:CE	2.38	0.53
1:A:170:SER:HB2	1:A:240:LYS:HE2	1.91	0.52
1:A:170:SER:HB3	1:A:240:LYS:HE2	1.91	0.51
1:B:212:LEU:HD21	1:B:248:LEU:HD13	1.92	0.51
1:B:223:GLN:NE2	1:B:324:ASN:CB	2.68	0.51
1:A:126:ILE:HG21	1:A:128:PHE:CE1	2.46	0.51
1:B:201:LEU:HD11	1:B:205:LYS:HE3	1.92	0.50
1:A:120:SER:HB3	1:A:153:ILE:HD11	1.96	0.48
1:A:367:THR:HB	1:A:370:ASP:OD2	2.13	0.47
1:B:265:LEU:HD23	1:B:310:ILE:HB	1.96	0.47
1:B:126:ILE:HG22	1:B:128:PHE:CE1	2.49	0.47
1:B:252:PHE:O	1:B:256:MET:HG3	2.15	0.47
1:B:103:ALA:HB1	1:B:167:PHE:CE2	2.50	0.46
1:A:121:LYS:HG2	1:A:153:ILE:CG2	2.45	0.46
1:B:253:VAL:HG21	1:B:299:LEU:CD2	2.45	0.46
1:A:161:ILE:HD13	1:A:164:MET:CE	2.45	0.46
1:B:160:ASN:HD22	1:B:160:ASN:C	2.20	0.45
1:B:273:VAL:HA	4:B:516:HOH:O	2.15	0.45
1:A:269:ALA:CB	1:A:274:VAL:HG13	2.46	0.45
1:B:178:ASP:CG	1:B:181:THR:HG23	2.38	0.44
1:A:121:LYS:HG2	1:A:153:ILE:HG21	1.99	0.44
1:B:103:ALA:HB1	1:B:167:PHE:HE2	1.83	0.44
1:A:282:SER:HB3	4:A:607:HOH:O	2.18	0.43
1:A:186:ARG:HA	1:A:186:ARG:NE	2.34	0.43
1:A:120:SER:HB3	1:A:153:ILE:CD1	2.50	0.41
1:A:323:ILE:HD12	3:A:500:JPJ:C24	2.50	0.41
1:B:416:GLY:O	1:B:419:ILE:HG12	2.21	0.41
1:A:243:TYR:CE2	1:A:247:SER:HB2	2.56	0.41
1:B:181:THR:O	1:B:187:TYR:HB2	2.21	0.41
1:A:323:ILE:HD11	3:A:500:JPJ:C19	2.51	0.40
1:B:98:ASP:HB2	1:B:124:VAL:HB	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	282/338 (83%)	272 (96%)	10 (4%)	0	100	100
1	B	277/338 (82%)	263 (95%)	14 (5%)	0	100	100
All	All	559/676 (83%)	535 (96%)	24 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	247/297 (83%)	232 (94%)	15 (6%)	26	22
1	B	244/297 (82%)	227 (93%)	17 (7%)	21	17
All	All	491/594 (83%)	459 (94%)	32 (6%)	24	20

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	97	GLU
1	A	105	ILE
1	A	124	VAL
1	A	137	ILE
1	A	162	LEU
1	A	178	ASP
1	A	188	ASN
1	A	218	ASN
1	A	226	LEU
1	A	227	LEU
1	A	238	LEU

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Mol	Chain	Res	Type
1	A	248	LEU
1	A	274	VAL
1	A	382	LEU
1	A	417	LEU
1	B	124	VAL
1	B	146	LYS
1	B	160	ASN
1	B	162	LEU
1	B	182	LYS
1	B	186	ARG
1	B	210	ASN
1	B	226	LEU
1	B	227	LEU
1	B	238	LEU
1	B	248	LEU
1	B	250	LYS
1	B	253	VAL
1	B	382	LEU
1	B	384	GLN
1	B	401	ARG
1	B	417	LEU

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	183	ASN
1	A	200	ASN
1	A	218	ASN
1	A	254	ASN
1	A	384	GLN
1	B	160	ASN
1	B	184	ASN
1	B	200	ASN
1	B	223	GLN
1	B	259	GLN
1	B	384	GLN

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	NAD	A	450	-	48,48,48	0.94	1 (2%)	73,73,73	1.88	13 (17%)
3	JPJ	A	500	-	26,26,26	0.93	2 (7%)	35,35,35	0.82	1 (2%)
2	NAD	B	450	-	48,48,48	0.92	2 (4%)	73,73,73	1.96	16 (21%)
3	JPJ	B	500	-	26,26,26	0.86	0	35,35,35	0.94	1 (2%)

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	NAD	A	450	-	-	0/30/62/62	0/3/5/5
3	JPJ	A	500	-	-	0/9/9/9	0/3/3/3
2	NAD	B	450	-	-	0/30/62/62	0/3/5/5
3	JPJ	B	500	-	-	0/9/9/9	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	450	NAD	C4A-N9A	-2.71	1.33	1.37
2	A	450	NAD	O4B-C1B	2.25	1.44	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	450	NAD	O4B-C1B	2.20	1.44	1.41
3	A	500	JPJ	C15-CL20	2.18	1.79	1.73
3	A	500	JPJ	C6-C1	2.14	1.41	1.38

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	450	NAD	N3A-C2A-N1A	-10.50	119.93	128.71
2	A	450	NAD	N3A-C2A-N1A	-8.44	121.65	128.71
2	A	450	NAD	O4B-C1B-N9A	5.66	113.71	108.44
2	B	450	NAD	C3N-C7N-N7N	4.08	122.42	117.77
2	B	450	NAD	N3A-C4A-N9A	3.94	132.55	125.43
2	A	450	NAD	N3A-C4A-N9A	3.92	132.51	125.43
2	B	450	NAD	C8A-N9A-C4A	3.85	109.83	106.90
2	A	450	NAD	O4D-C1D-N1N	3.73	111.77	107.95
2	A	450	NAD	C3N-C7N-N7N	3.69	121.97	117.77
2	B	450	NAD	O3-PN-O1N	3.65	117.55	108.83
2	B	450	NAD	C4B-O4B-C1B	-3.32	106.14	109.75
2	A	450	NAD	C4B-O4B-C1B	-3.25	106.22	109.75
2	A	450	NAD	C2D-C1D-N1N	3.04	119.00	113.86
2	B	450	NAD	O7N-C7N-N7N	-2.67	118.74	122.59
2	B	450	NAD	O3B-C3B-C4B	-2.55	103.55	111.08
3	B	500	JPJ	C7-C18-C28	2.39	120.78	113.28
2	B	450	NAD	C6N-N1N-C1D	-2.37	113.46	119.33
2	B	450	NAD	C1B-N9A-C4A	-2.35	122.58	126.64
2	A	450	NAD	O2N-PN-O3	-2.35	102.46	108.79
2	A	450	NAD	C5A-C4A-N3A	-2.33	120.62	125.70
2	A	450	NAD	O4D-C1D-C2D	-2.28	103.28	106.77
2	B	450	NAD	N7A-C8A-N9A	-2.23	108.04	114.36
2	A	450	NAD	C8A-N9A-C4A	2.18	108.56	106.90
2	B	450	NAD	C5A-C4A-N3A	-2.17	120.98	125.70
2	B	450	NAD	O4D-C1D-C2D	-2.10	103.55	106.77
2	B	450	NAD	C2B-C3B-C4B	2.10	106.83	102.65
2	A	450	NAD	PN-O5D-C5D	2.09	127.47	120.24
2	B	450	NAD	C2A-N3A-C4A	2.08	119.93	114.01
2	B	450	NAD	C2A-N1A-C6A	2.08	122.52	118.77
3	A	500	JPJ	O13-C2-C1	2.07	120.55	116.33
2	A	450	NAD	O3-PN-O1N	2.01	113.62	108.83

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, 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	286/338 (84%)	0.44	32 (11%) 6 6	24, 35, 64, 81	0
1	B	283/338 (83%)	0.45	33 (11%) 5 6	24, 37, 67, 81	0
All	All	569/676 (84%)	0.45	65 (11%) 6 6	24, 36, 67, 81	0

All (65) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	156	ASP	5.8
1	B	152	ILE	5.8
1	B	149	ASN	5.2
1	A	181	THR	5.2
1	A	177	ILE	5.1
1	B	153	ILE	4.9
1	B	142	TYR	4.4
1	B	148	ASP	4.4
1	A	154	ASP	4.3
1	A	368	PHE	4.2
1	A	183	ASN	4.2
1	B	213	VAL	4.1
1	B	368	PHE	4.1
1	A	153	ILE	4.1
1	B	146	LYS	4.0
1	A	155	LYS	4.0
1	B	144	ASN	4.0
1	B	143	LYS	3.9
1	B	97	GLU	3.9
1	A	180	GLU	3.9
1	B	145	GLY	3.9
1	A	186	ARG	3.7
1	B	179	GLU	3.5
1	B	102	ILE	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	216	LEU	3.1
1	A	179	GLU	3.1
1	A	178	ASP	3.0
1	A	321	THR	3.0
1	B	103	ALA	3.0
1	B	212	LEU	2.9
1	A	185	LYS	2.9
1	A	318	ARG	2.9
1	A	157	LYS	2.9
1	B	137	ILE	2.8
1	A	175	ASN	2.7
1	B	189	MET	2.7
1	B	150	ASP	2.6
1	A	367	THR	2.6
1	A	102	ILE	2.6
1	B	263	ILE	2.6
1	A	188	ASN	2.5
1	A	103	ALA	2.5
1	A	97	GLU	2.5
1	A	189	MET	2.5
1	B	158	LYS	2.4
1	B	324	ASN	2.4
1	B	262	ILE	2.4
1	B	104	GLY	2.4
1	B	207	GLY	2.4
1	A	248	LEU	2.3
1	A	223	GLN	2.2
1	A	140	LYS	2.2
1	A	288	LEU	2.2
1	A	144	ASN	2.2
1	A	371	TYR	2.2
1	B	264	SER	2.2
1	A	152	ILE	2.1
1	B	214	HIS	2.1
1	A	182	LYS	2.1
1	B	141	ASN	2.1
1	B	160	ASN	2.1
1	B	215	SER	2.0
1	A	258	PRO	2.0
1	B	147	PHE	2.0
1	B	371	TYR	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
2	NAD	B	450	44/44	0.13	-0.02	27,33,41,44	0
3	JPJ	B	500	24/24	0.11	-0.21	31,35,51,52	0
3	JPJ	A	500	24/24	0.10	-0.52	32,36,47,50	0
2	NAD	A	450	44/44	0.09	-0.79	28,37,42,44	0

6.5 Other polymers ⓘ

There are no such residues in this entry.