



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 04:54 AM GMT

PDB ID : 2OOS  
Title : Crystal structure of plasmodium falciparum enoyl ACP reductase with triclosan reductase  
Authors : Tsai, H.  
Deposited on : 2007-01-26  
Resolution : 2.10 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 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
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) : trunk26865

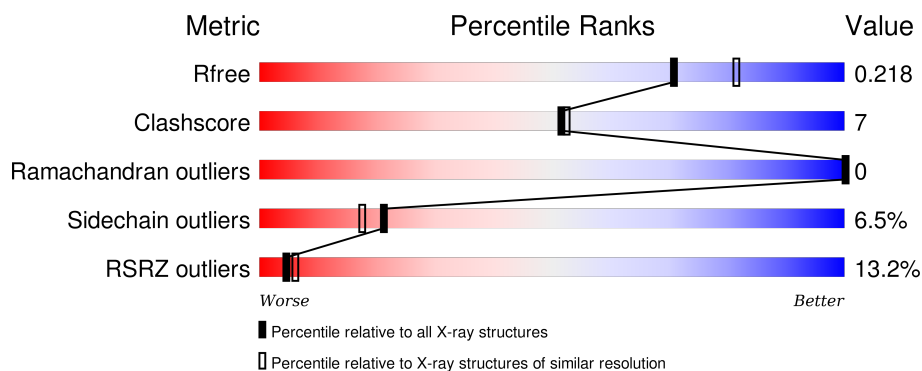
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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))
$R_{free}$	91344	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (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  $\geq 3$ , 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	338	<div> <div>11%</div> <div>71%</div> <div>12%</div> <div>•</div> <div>15%</div> </div>
1	B	338	<div> <div>12%</div> <div>69%</div> <div>12%</div> <div>•</div> <div>16%</div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4805 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 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:

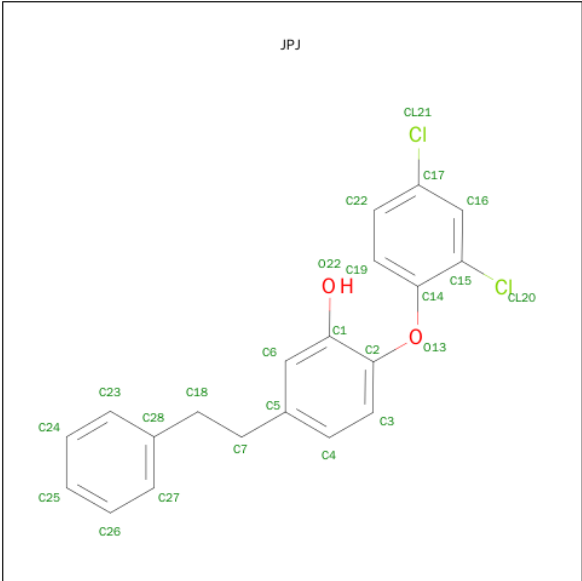
Chain	Residue	Modelled	Actual	Comment	Reference
A	88	MET	-	CLONING ARTIFACT	UNP Q9BH77
A	89	VAL	-	CLONING ARTIFACT	UNP Q9BH77
A	90	HIS	-	EXPRESSION TAG	UNP Q9BH77
A	91	HIS	-	EXPRESSION TAG	UNP Q9BH77
A	92	HIS	-	EXPRESSION TAG	UNP Q9BH77
A	93	HIS	-	EXPRESSION TAG	UNP Q9BH77
A	94	HIS	-	EXPRESSION TAG	UNP 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: C<sub>21</sub>H<sub>27</sub>N<sub>7</sub>O<sub>14</sub>P<sub>2</sub>).



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: C<sub>20</sub>H<sub>16</sub>Cl<sub>2</sub>O<sub>2</sub>).



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		

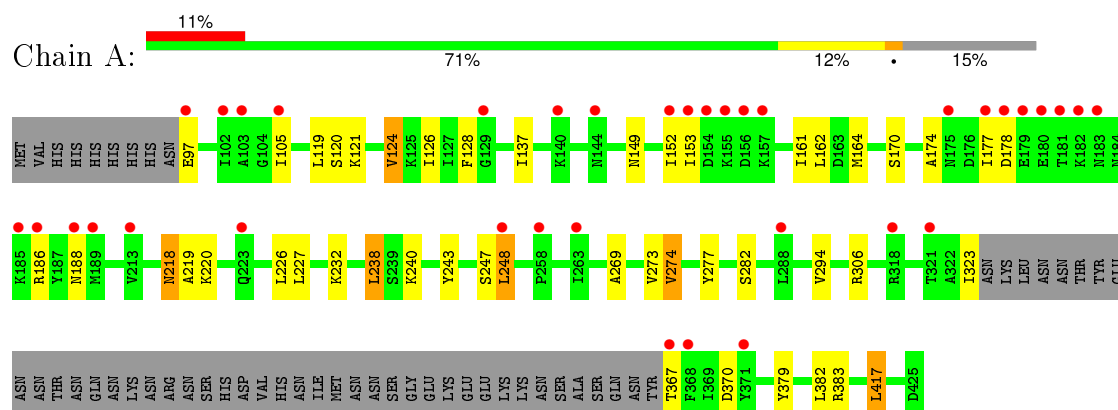
- Molecule 4 is water.

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

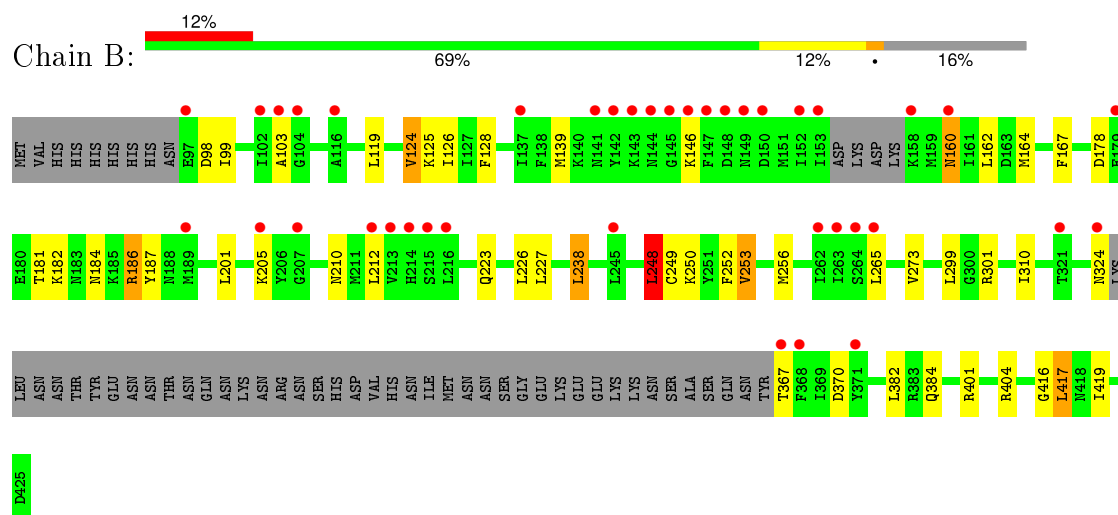
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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



#### • Molecule 1: Enoyl-acyl carrier reductase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.94 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.192 , 0.227 0.184 , 0.218	Depositor DCC
$R_{free}$ test set	2160 reflections (5.32%)	DCC
Wilson B-factor (Å <sup>2</sup> )	38.9	Xtriage
Anisotropy	0.189	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 43.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	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 <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 3.53% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: 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 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	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

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 7.

All (63) 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: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
1:B:178:ASP:OD1	1:B:181:THR:HG23	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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%)	23	19
1	B	244/297 (82%)	227 (93%)	17 (7%)	19	15
All	All	491/594 (83%)	459 (94%)	32 (6%)	21	17

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

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Mol	Chain	Res	Type
1	A	226	LEU
1	A	227	LEU
1	A	238	LEU
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 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 ⓘ

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	-	38,48,48	0.98	3 (7%)	47,73,73	1.96	5 (10%)
3	JPJ	A	500	-	26,26,26	0.96	2 (7%)	35,35,35	0.85	1 (2%)
2	NAD	B	450	-	38,48,48	0.89	1 (2%)	47,73,73	2.20	9 (19%)
3	JPJ	B	500	-	26,26,26	0.91	0	35,35,35	0.95	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	-	-	0/22/62/62	0/5/5/5
3	JPJ	A	500	-	-	0/9/9/9	0/3/3/3
2	NAD	B	450	-	-	0/22/62/62	0/5/5/5
3	JPJ	B	500	-	-	0/9/9/9	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	450	NAD	O7N-C7N	-2.01	1.19	1.24
3	A	500	JPJ	C6-C1	2.15	1.41	1.38
2	A	450	NAD	C2A-N3A	2.17	1.36	1.32
3	A	500	JPJ	C15-CL20	2.27	1.79	1.73
2	B	450	NAD	O4B-C1B	2.79	1.44	1.41
2	A	450	NAD	O4B-C1B	2.84	1.44	1.41

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	450	NAD	N3A-C2A-N1A	-11.71	119.93	128.89
2	A	450	NAD	N3A-C2A-N1A	-9.46	121.65	128.89
2	B	450	NAD	C4B-O4B-C1B	-3.25	106.14	109.72
2	A	450	NAD	C4B-O4B-C1B	-3.18	106.22	109.72
2	B	450	NAD	C1B-N9A-C4A	-2.89	122.58	126.94
2	B	450	NAD	O7N-C7N-N7N	-2.74	118.74	122.59
2	B	450	NAD	O3B-C3B-C4B	-2.50	103.55	111.05
2	B	450	NAD	O5B-C5B-C4B	-2.00	101.74	109.12
2	B	450	NAD	C2B-C3B-C4B	2.05	106.83	102.61
2	B	450	NAD	C2A-N1A-C6A	2.10	122.52	118.77
3	A	500	JPJ	O13-C2-C1	2.26	120.55	116.12
3	B	500	JPJ	C7-C18-C28	2.28	120.78	113.27
2	A	450	NAD	O4B-C1B-N9A	2.68	113.71	108.10
2	A	450	NAD	O4D-C1D-N1N	3.31	111.77	108.13
2	A	450	NAD	C3N-C7N-N7N	3.79	121.97	117.82
2	B	450	NAD	C3N-C7N-N7N	4.20	122.42	117.82

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	500	JPJ	2	0

## 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	286/338 (84%)	0.56	36 (12%) 5 6	24, 35, 64, 81	0
1	B	283/338 (83%)	0.58	39 (13%) 4 5	24, 37, 67, 81	0
All	All	569/676 (84%)	0.57	75 (13%) 4 6	24, 36, 67, 81	0

All (75) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	153	ILE	6.7
1	B	152	ILE	6.5
1	A	156	ASP	6.3
1	A	177	ILE	6.1
1	A	181	THR	6.0
1	B	149	ASN	5.3
1	B	213	VAL	5.0
1	A	368	PHE	5.0
1	A	154	ASP	4.7
1	A	155	LYS	4.7
1	B	142	TYR	4.6
1	B	148	ASP	4.6
1	B	368	PHE	4.4
1	A	186	ARG	4.3
1	B	143	LYS	4.3
1	A	153	ILE	4.3
1	B	145	GLY	4.3
1	A	180	GLU	4.3
1	A	183	ASN	4.2
1	B	144	ASN	4.0
1	B	146	LYS	4.0
1	B	97	GLU	4.0
1	B	102	ILE	3.9
1	B	216	LEU	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	321	THR	3.7
1	B	150	ASP	3.7
1	A	178	ASP	3.6
1	B	103	ALA	3.5
1	B	179	GLU	3.5
1	B	212	LEU	3.5
1	B	137	ILE	3.5
1	A	157	LYS	3.4
1	B	263	ILE	3.3
1	A	103	ALA	3.2
1	A	318	ARG	3.0
1	A	189	MET	3.0
1	A	185	LYS	3.0
1	A	102	ILE	2.9
1	A	175	ASN	2.9
1	B	189	MET	2.9
1	A	179	GLU	2.9
1	A	223	GLN	2.8
1	A	248	LEU	2.8
1	B	207	GLY	2.8
1	B	158	LYS	2.8
1	A	188	ASN	2.8
1	B	104	GLY	2.8
1	A	367	THR	2.8
1	B	141	ASN	2.7
1	B	262	ILE	2.6
1	B	324	ASN	2.6
1	A	144	ASN	2.4
1	B	215	SER	2.3
1	A	371	TYR	2.3
1	A	140	LYS	2.3
1	B	264	SER	2.3
1	B	214	HIS	2.3
1	B	245	LEU	2.3
1	B	160	ASN	2.3
1	B	265	LEU	2.3
1	A	182	LYS	2.3
1	A	97	GLU	2.2
1	B	147	PHE	2.2
1	B	367	THR	2.2
1	B	321	THR	2.2
1	A	263	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	213	VAL	2.1
1	B	205	LYS	2.1
1	B	371	TYR	2.1
1	A	152	ILE	2.1
1	A	288	LEU	2.1
1	A	258	PRO	2.1
1	A	129	GLY	2.0
1	A	105	ILE	2.0
1	B	116	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
2	NAD	B	450	44/44	0.97	0.13	-0.11	27,33,41,44	0
3	JPJ	B	500	24/24	0.95	0.11	-0.13	31,35,51,52	0
3	JPJ	A	500	24/24	0.96	0.12	-0.32	32,36,47,50	0
2	NAD	A	450	44/44	0.97	0.10	-0.78	28,37,42,44	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.