



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 01:44 PM GMT

PDB ID : 1LPF  
Title : THREE-DIMENSIONAL STRUCTURE OF LIPOAMIDE DEHYDROGENASE FROM PSEUDOMONAS FLUORESCENS AT 2.8 ANGSTROMS RESOLUTION. ANALYSIS OF REDOX AND THERMOSTABILITY PROPERTIES  
Authors : Mattevi, A.; Hol, W.  
Deposited on : 1992-10-26  
Resolution : 2.80 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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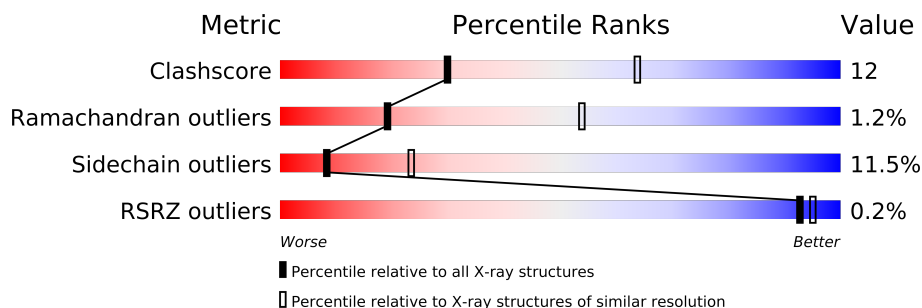
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.80 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	2295 (2.80-2.80)
Ramachandran outliers	78287	2252 (2.80-2.80)
Sidechain outliers	78261	2254 (2.80-2.80)
RSRZ outliers	66119	1802 (2.80-2.80)

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	477	
1	B	477	

## 2 Entry composition i

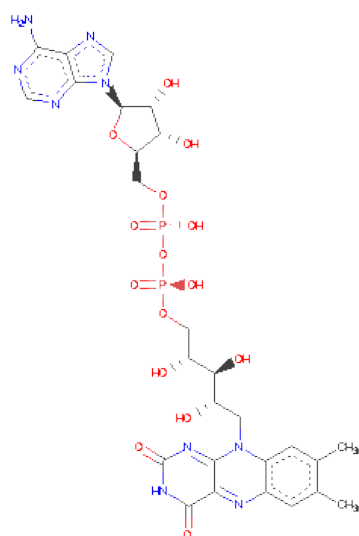
There are 2 unique types of molecules in this entry. The entry contains 6962 atoms, of which 0 are hydrogen and 0 are deuterium.

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 DIHYDROLIPOAMIDE DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	472	Total	C	N	O	S	0	0	0
			3428	2172	588	656	12			
1	B	472	Total	C	N	O	S	0	0	0
			3428	2172	588	656	12			

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula:  $C_{27}H_{33}N_9O_{15}P_2$ ).



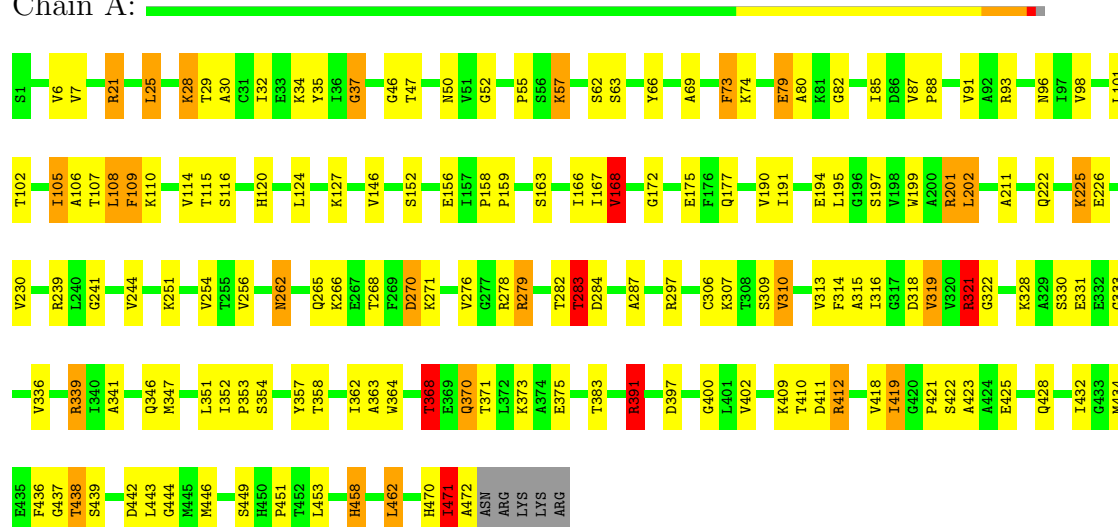
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

### 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.

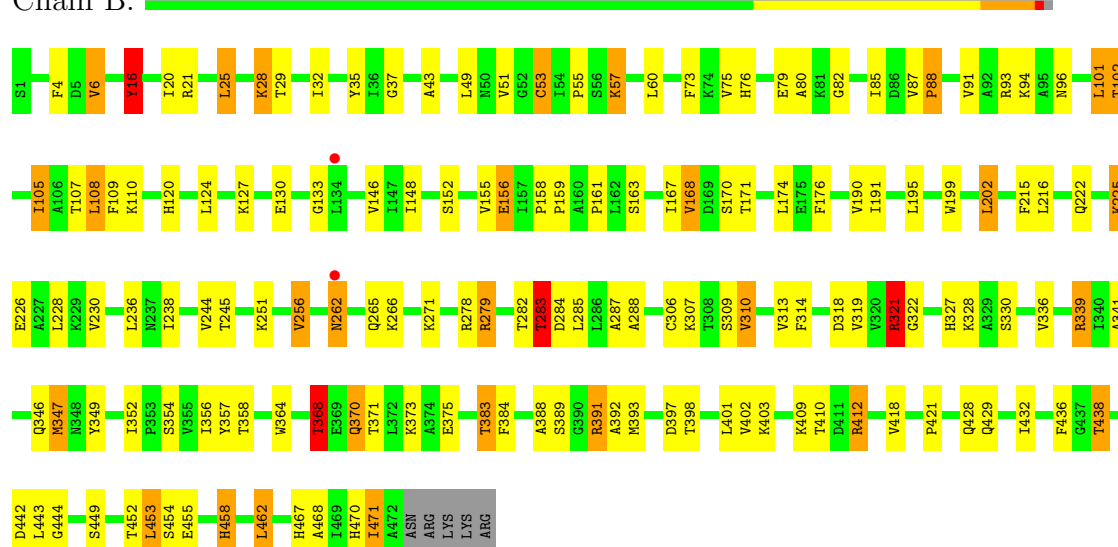
#### • Molecule 1: DIHYDROLIPOAMIDE DEHYDROGENASE

Chain A:



#### • Molecule 1: DIHYDROLIPOAMIDE DEHYDROGENASE

Chain B:



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	113.60Å 66.40Å 164.30Å 90.00° 99.20° 90.00°	Depositor
Resolution (Å)	10.00 – 2.80 15.05 – 2.80	Depositor EDS
% Data completeness (in resolution range)	(Not available) (10.00-2.80) 78.8 (15.05-2.80)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.22 (at 2.81Å)	Xtriage
Refinement program	X-PLOR	Depositor
R, $R_{free}$	0.192 , (Not available) 0.188 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	46.5	Xtriage
Anisotropy	0.285	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.24 , 28.2	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	1 of 23543 reflections (0.004%)	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	6962	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.40% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

## 5 Model quality i

### 5.1 Standard geometry i

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	1.04	0/3480	1.64	46/4725 (1.0%)
1	B	1.01	2/3480 (0.1%)	1.65	36/4725 (0.8%)
All	All	1.03	2/6960 (0.0%)	1.65	82/9450 (0.9%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	458	HIS	CA-CB	-5.63	1.41	1.53
1	B	453	LEU	CA-CB	-5.14	1.42	1.53

All (82) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	339	ARG	NE-CZ-NH2	-10.51	115.05	120.30
1	A	391	ARG	NE-CZ-NH1	9.53	125.06	120.30
1	B	278	ARG	NE-CZ-NH2	-8.84	115.88	120.30
1	B	321	ARG	NE-CZ-NH1	8.31	124.46	120.30
1	A	434	MET	CG-SD-CE	-8.23	87.04	100.20
1	A	66	TYR	CB-CG-CD2	-8.09	116.14	121.00
1	A	364	TRP	CD1-CG-CD2	8.03	112.73	106.30
1	B	364	TRP	CG-CD2-CE3	7.87	140.99	133.90
1	A	364	TRP	CE2-CD2-CG	-7.79	101.07	107.30
1	A	321	ARG	NE-CZ-NH1	7.64	124.12	120.30
1	B	93	ARG	NE-CZ-NH2	-7.63	116.48	120.30
1	B	339	ARG	NE-CZ-NH1	7.63	124.11	120.30
1	A	397	ASP	CB-CG-OD2	-7.23	111.79	118.30
1	A	278	ARG	NE-CZ-NH2	-7.17	116.71	120.30
1	B	364	TRP	CE2-CD2-CG	-7.04	101.67	107.30
1	B	364	TRP	CD1-CG-CD2	7.02	111.91	106.30
1	B	391	ARG	NE-CZ-NH1	6.94	123.77	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	16	TYR	CB-CG-CD2	-6.83	116.90	121.00
1	A	276	VAL	CA-CB-CG2	-6.74	100.78	110.90
1	A	339	ARG	NE-CZ-NH2	-6.74	116.93	120.30
1	A	168	VAL	N-CA-CB	-6.72	96.72	111.50
1	B	155	VAL	CA-CB-CG2	-6.72	100.83	110.90
1	A	98	VAL	CG1-CB-CG2	-6.70	100.17	110.90
1	B	393	MET	CA-CB-CG	-6.65	101.99	113.30
1	A	201	ARG	NE-CZ-NH1	6.62	123.61	120.30
1	A	199	TRP	CD1-CG-CD2	6.60	111.58	106.30
1	B	368	THR	N-CA-CB	-6.60	97.77	110.30
1	A	279	ARG	NE-CZ-NH1	6.58	123.59	120.30
1	A	199	TRP	CE2-CD2-CG	-6.52	102.08	107.30
1	B	279	ARG	NE-CZ-NH1	6.48	123.54	120.30
1	B	199	TRP	CE2-CD2-CG	-6.47	102.13	107.30
1	B	168	VAL	N-CA-CB	-6.45	97.31	111.50
1	B	364	TRP	CB-CG-CD1	-6.39	118.69	127.00
1	B	199	TRP	CD1-CG-CD2	6.36	111.39	106.30
1	B	102	THR	N-CA-CB	-6.34	98.25	110.30
1	A	225	LYS	CA-CB-CG	6.29	127.24	113.40
1	B	278	ARG	NE-CZ-NH1	6.25	123.43	120.30
1	A	283	THR	CA-C-N	6.24	130.93	117.20
1	A	199	TRP	CG-CD2-CE3	6.22	139.50	133.90
1	A	166	ILE	CG1-CB-CG2	-6.21	97.73	111.40
1	B	283	THR	CA-CB-CG2	6.18	121.05	112.40
1	B	256	VAL	CA-CB-CG2	-6.04	101.84	110.90
1	B	467	HIS	N-CA-C	6.00	127.21	111.00
1	A	102	THR	N-CA-CB	-5.99	98.91	110.30
1	A	270	ASP	CB-CG-OD2	-5.96	112.94	118.30
1	B	127	LYS	CB-CG-CD	-5.94	96.16	111.60
1	A	251	LYS	CA-CB-CG	5.83	126.23	113.40
1	B	228	LEU	O-C-N	5.80	131.98	122.70
1	A	7	VAL	CG1-CB-CG2	-5.79	101.63	110.90
1	B	397	ASP	CB-CG-OD2	-5.77	113.11	118.30
1	A	437	GLY	CA-C-O	-5.69	110.36	120.60
1	A	73	PHE	CB-CG-CD2	-5.67	116.83	120.80
1	A	364	TRP	CG-CD2-CE3	5.67	139.00	133.90
1	A	268	THR	O-C-N	-5.58	113.77	122.70
1	A	276	VAL	CA-CB-CG1	5.54	119.20	110.90
1	A	368	THR	N-CA-CB	-5.50	99.84	110.30
1	A	449	SER	CB-CA-C	-5.49	99.67	110.10
1	A	175	GLU	N-CA-CB	-5.39	100.91	110.60
1	A	283	THR	CA-CB-CG2	5.38	119.94	112.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	239	ARG	NE-CZ-NH2	-5.35	117.62	120.30
1	B	251	LYS	CA-CB-CG	5.34	125.14	113.40
1	A	319	VAL	CB-CA-C	-5.33	101.28	111.40
1	B	306	CYS	CA-CB-SG	-5.32	104.43	114.00
1	A	114	VAL	CA-C-N	-5.31	105.51	117.20
1	A	402	VAL	CG1-CB-CG2	-5.30	102.41	110.90
1	B	236	LEU	CA-CB-CG	5.30	127.49	115.30
1	A	339	ARG	NE-CZ-NH1	5.30	122.95	120.30
1	A	336	VAL	CG1-CB-CG2	-5.29	102.44	110.90
1	B	109	PHE	CB-CG-CD2	-5.20	117.16	120.80
1	A	270	ASP	CB-CG-OD1	5.19	122.97	118.30
1	A	127	LYS	CB-CG-CD	-5.18	98.12	111.60
1	A	412	ARG	NE-CZ-NH1	5.18	122.89	120.30
1	A	315	ALA	CA-C-N	5.17	128.57	117.20
1	B	336	VAL	CG1-CB-CG2	-5.17	102.63	110.90
1	A	297	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	A	458	HIS	CG-CD2-NE2	-5.11	99.49	109.20
1	B	283	THR	CA-C-N	5.10	128.43	117.20
1	B	91	VAL	CG1-CB-CG2	-5.09	102.75	110.90
1	B	364	TRP	CA-CB-CG	5.07	123.32	113.70
1	B	412	ARG	NE-CZ-NH1	5.04	122.82	120.30
1	A	362	ILE	CG1-CB-CG2	-5.03	100.33	111.40
1	B	225	LYS	CA-CB-CG	5.03	124.47	113.40

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	3428	0	3470	92	0
1	B	3428	0	3470	90	0
2	A	53	0	31	1	0
2	B	53	0	31	2	0
All	All	6962	0	7002	169	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 12.

All (169) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:262:ASN:HD22	1:B:262:ASN:H	1.12	0.97
1:B:262:ASN:HD22	1:B:262:ASN:N	1.63	0.94
1:A:262:ASN:N	1:A:262:ASN:HD22	1.65	0.93
1:A:262:ASN:H	1:A:262:ASN:ND2	1.69	0.90
1:A:262:ASN:HD22	1:A:262:ASN:H	0.88	0.85
1:B:262:ASN:ND2	1:B:262:ASN:H	1.83	0.76
1:B:146:VAL:HB	1:B:313:VAL:HG22	1.68	0.74
1:B:428:GLN:O	1:B:432:ILE:HG13	1.89	0.73
1:A:438:THR:HG23	1:B:436:PHE:CZ	2.23	0.73
1:A:146:VAL:HB	1:A:313:VAL:HG22	1.69	0.72
1:A:438:THR:HG23	1:B:436:PHE:HZ	1.54	0.71
1:A:436:PHE:CZ	1:B:438:THR:HG23	2.27	0.68
1:A:438:THR:HG21	1:A:443:LEU:HG	1.75	0.67
1:A:80:ALA:HB1	1:B:80:ALA:HB1	1.77	0.66
1:A:391:ARG:HG3	1:A:391:ARG:HH11	1.60	0.65
1:A:436:PHE:HZ	1:B:438:THR:HG23	1.62	0.65
1:B:158:PRO:HG2	1:B:159:PRO:HD3	1.79	0.64
1:A:158:PRO:HG2	1:A:159:PRO:HD3	1.81	0.62
1:A:52:GLY:O	1:A:55:PRO:HD2	1.99	0.62
1:B:370:GLN:NE2	1:B:370:GLN:H	1.97	0.62
1:A:88:PRO:HG3	1:A:177:GLN:HG3	1.80	0.62
1:B:35:TYR:HD2	1:B:43:ALA:HB3	1.65	0.62
1:A:310:VAL:HG22	1:A:313:VAL:HB	1.80	0.61
1:B:262:ASN:ND2	1:B:262:ASN:N	2.37	0.60
1:A:438:THR:HG22	1:A:442:ASP:HB2	1.83	0.60
1:A:351:LEU:O	1:A:353:PRO:HD3	2.02	0.59
1:B:347:MET:HG2	1:B:349:TYR:CE2	2.37	0.59
1:A:163:SER:H	1:A:167:ILE:HB	1.69	0.58
1:A:373:LYS:HA	1:A:373:LYS:HE2	1.87	0.56
1:B:307:LYS:HG2	1:B:314:PHE:HE1	1.71	0.56
1:B:87:VAL:HB	1:B:88:PRO:HD3	1.87	0.56
1:B:373:LYS:HE2	1:B:373:LYS:HA	1.87	0.56
1:A:226:GLU:O	1:A:230:VAL:HG23	2.05	0.56
1:A:421:PRO:HB2	1:A:453:LEU:HD13	1.87	0.56
1:B:310:VAL:HG22	1:B:313:VAL:HB	1.88	0.56
1:A:87:VAL:O	1:A:91:VAL:HG23	2.05	0.56
1:A:322:GLY:HA3	1:A:328:LYS:HE3	1.88	0.56
1:A:428:GLN:O	1:A:432:ILE:HG13	2.05	0.56
1:B:244:VAL:HG13	1:B:256:VAL:HG13	1.87	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:368:THR:HG22	1:A:371:THR:OG1	2.06	0.56
1:B:438:THR:HG22	1:B:442:ASP:HB2	1.88	0.55
1:B:438:THR:HG21	1:B:443:LEU:HG	1.88	0.55
1:A:28:LYS:HZ1	1:A:29:THR:H	1.53	0.55
1:A:244:VAL:HG13	1:A:256:VAL:HG13	1.88	0.55
1:B:444:GLY:O	1:B:458:HIS:HE1	1.89	0.54
1:B:51:VAL:CG1	1:B:171:THR:HG23	2.38	0.54
1:B:124:LEU:HD23	1:B:287:ALA:HB2	1.89	0.54
1:B:120:HIS:HE1	1:B:284:ASP:O	1.91	0.53
1:B:4:PHE:HD1	1:B:28:LYS:HG3	1.74	0.52
1:B:55:PRO:HB3	1:B:94:LYS:HD2	1.90	0.52
1:B:347:MET:HG2	1:B:349:TYR:CZ	2.45	0.52
1:A:370:GLN:H	1:A:370:GLN:NE2	2.07	0.52
1:A:316:ILE:HD12	1:A:333:GLY:HA2	1.92	0.50
1:B:368:THR:HG22	1:B:371:THR:OG1	2.12	0.50
1:B:384:PHE:CZ	1:B:388:ALA:HB3	2.47	0.50
1:A:87:VAL:HB	1:A:88:PRO:HD3	1.92	0.50
1:B:163:SER:H	1:B:167:ILE:HB	1.77	0.49
1:B:191:ILE:O	1:B:195:LEU:HD23	2.12	0.49
1:A:106:ALA:O	1:A:109:PHE:HB2	2.12	0.49
1:A:34:LYS:NZ	1:A:120:HIS:HD2	2.10	0.49
1:B:35:TYR:CD2	1:B:43:ALA:HB3	2.46	0.49
1:B:148:ILE:HG21	1:B:285:LEU:HD21	1.92	0.49
1:B:391:ARG:HH11	1:B:391:ARG:HG3	1.78	0.48
1:A:411:ASP:O	1:A:439:SER:HA	2.14	0.48
1:B:105:ILE:HA	1:B:108:LEU:HB2	1.96	0.48
1:A:438:THR:CG2	1:B:436:PHE:HZ	2.26	0.48
1:A:120:HIS:HE1	1:A:284:ASP:O	1.97	0.48
1:B:156:GLU:HB2	1:B:279:ARG:HH22	1.79	0.48
1:A:339:ARG:HH21	1:A:346:GLN:NE2	2.12	0.48
1:A:30:ALA:HA	1:A:115:THR:O	2.15	0.47
1:A:93:ARG:HD3	1:B:75:VAL:O	2.14	0.47
1:B:322:GLY:HA3	1:B:328:LYS:HE3	1.96	0.47
1:B:226:GLU:O	1:B:230:VAL:HG23	2.15	0.47
1:A:25:LEU:HG	1:A:341:ALA:CB	2.45	0.47
1:B:32:ILE:HG22	2:B:480:FAD:H2A	1.96	0.47
1:B:60:LEU:HD13	1:B:357:TYR:O	2.14	0.47
1:B:215:PHE:CE2	1:B:216:LEU:HD12	2.50	0.47
1:A:57:LYS:HD3	1:A:57:LYS:HA	1.71	0.47
1:A:74:LYS:HE3	1:A:79:GLU:OE2	2.13	0.46
1:A:62:SER:HB3	1:B:76:HIS:HB3	1.97	0.46
1:B:421:PRO:HB2	1:B:453:LEU:HD13	1.97	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:211:ALA:O	1:A:241:GLY:HA2	2.16	0.46
1:B:371:THR:O	1:B:375:GLU:HG3	2.16	0.46
1:A:307:LYS:HG2	1:A:314:PHE:HE1	1.81	0.46
1:A:262:ASN:N	1:A:262:ASN:ND2	2.39	0.45
1:B:191:ILE:HG22	1:B:195:LEU:HD23	1.98	0.45
1:A:425:GLU:HG3	1:B:454:SER:OG	2.16	0.45
1:A:57:LYS:HD2	1:A:357:TYR:CG	2.52	0.45
1:B:462:LEU:HB3	1:B:468:ALA:HA	1.99	0.45
1:B:470:HIS:O	1:B:471:ILE:HG23	2.16	0.45
1:B:158:PRO:O	1:B:161:PRO:HG3	2.16	0.45
1:A:339:ARG:NH2	1:A:346:GLN:HE22	2.14	0.45
1:B:410:THR:HG21	1:B:412:ARG:NH2	2.32	0.45
1:A:432:ILE:CD1	1:B:429:GLN:HB3	2.47	0.45
1:B:6:VAL:HB	1:B:29:THR:HG23	1.98	0.45
1:B:53:CYS:O	1:B:57:LYS:HE2	2.16	0.45
1:B:120:HIS:CE1	1:B:284:ASP:O	2.69	0.45
1:A:470:HIS:O	1:A:471:ILE:HG23	2.17	0.45
1:A:354:SER:O	1:A:363:ALA:HA	2.16	0.45
1:B:16:TYR:O	1:B:20:ILE:HG13	2.17	0.45
1:B:170:SER:HB3	2:B:480:FAD:HM71	1.98	0.45
1:A:190:VAL:O	1:A:194:GLU:HG3	2.16	0.44
1:A:28:LYS:HA	1:A:28:LYS:HZ2	1.82	0.44
1:A:444:GLY:O	1:A:458:HIS:HE1	2.00	0.44
1:B:49:LEU:HD21	1:B:101:LEU:HB3	1.99	0.44
1:B:94:LYS:NZ	1:B:174:LEU:O	2.51	0.44
1:B:57:LYS:HD3	1:B:57:LYS:HA	1.55	0.44
1:B:190:VAL:HG22	1:B:356:ILE:HG12	2.00	0.44
1:A:462:LEU:HA	1:A:462:LEU:HD12	1.82	0.44
1:A:152:SER:HB3	1:A:318:ASP:HB3	2.00	0.44
1:A:168:VAL:HG22	1:A:172:GLY:HA3	2.00	0.44
1:B:28:LYS:HZ1	1:B:29:THR:H	1.66	0.44
1:A:32:ILE:HG22	2:A:480:FAD:H2A	1.99	0.44
1:A:35:TYR:CE2	1:A:37:GLY:HA2	2.53	0.43
1:B:215:PHE:HE1	1:B:238:ILE:HD13	1.83	0.43
1:B:110:LYS:HA	1:B:110:LYS:HD3	1.88	0.43
1:B:124:LEU:HD11	1:B:130:GLU:HB2	1.99	0.43
1:A:451:PRO:HD3	1:B:53:CYS:HB3	1.99	0.43
1:A:471:ILE:O	1:A:472:ALA:HB2	2.18	0.43
1:A:202:LEU:HD23	1:A:202:LEU:N	2.33	0.43
1:B:339:ARG:HH21	1:B:346:GLN:NE2	2.16	0.43
1:A:46:GLY:O	1:A:50:ASN:HB2	2.18	0.43
1:A:105:ILE:HA	1:A:108:LEU:HB2	2.01	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:339:ARG:NH2	1:B:346:GLN:HE22	2.17	0.43
1:A:442:ASP:O	1:A:446:MET:HG3	2.19	0.43
1:B:159:PRO:HB3	1:B:245:THR:O	2.18	0.43
1:A:63:SER:HB3	1:A:202:LEU:HD21	2.01	0.43
1:A:438:THR:HG22	1:A:442:ASP:CB	2.48	0.43
1:A:371:THR:O	1:A:375:GLU:HG3	2.18	0.43
1:A:436:PHE:HZ	1:B:438:THR:CG2	2.28	0.42
1:A:85:ILE:HG12	1:A:202:LEU:HD13	2.01	0.42
1:B:85:ILE:HG12	1:B:202:LEU:CD1	2.48	0.42
1:A:156:GLU:HB2	1:A:279:ARG:HH22	1.84	0.42
1:B:321:ARG:H	1:B:321:ARG:HG3	1.70	0.42
1:A:400:GLY:HA3	1:A:419:ILE:O	2.19	0.42
1:B:176:PHE:CZ	1:B:271:LYS:HG2	2.54	0.42
1:A:306:CYS:SG	1:A:321:ARG:NH2	2.93	0.42
1:B:455:GLU:O	1:B:458:HIS:HB3	2.19	0.42
1:B:402:VAL:HG12	1:B:403:LYS:N	2.34	0.42
1:B:25:LEU:HG	1:B:341:ALA:CB	2.49	0.42
1:B:443:LEU:HA	1:B:443:LEU:HD23	1.76	0.42
1:A:331:GLU:HB3	1:A:347:MET:SD	2.60	0.42
1:A:191:ILE:HG22	1:A:195:LEU:HD23	2.01	0.42
1:A:443:LEU:HD23	1:A:443:LEU:HA	1.84	0.41
1:B:49:LEU:HG	1:B:49:LEU:O	2.20	0.41
1:A:191:ILE:O	1:A:195:LEU:HD23	2.20	0.41
1:A:421:PRO:HB2	1:A:453:LEU:CD1	2.49	0.41
1:A:34:LYS:HZ3	1:A:120:HIS:CD2	2.39	0.41
1:A:197:SER:O	1:A:201:ARG:HD3	2.20	0.41
1:B:383:THR:HG23	1:B:401:LEU:HD12	2.03	0.41
1:B:307:LYS:HG2	1:B:314:PHE:CE1	2.52	0.41
1:B:51:VAL:HG11	1:B:171:THR:HG23	2.02	0.41
1:A:69:ALA:HA	1:A:73:PHE:CG	2.54	0.41
1:B:389:SER:HB3	1:B:392:ALA:HB3	2.02	0.41
1:A:270:ASP:O	1:A:271:LYS:HD2	2.21	0.41
1:A:307:LYS:HG2	1:A:314:PHE:CE1	2.56	0.41
1:A:410:THR:HG21	1:A:412:ARG:NH2	2.35	0.41
1:B:256:VAL:O	1:B:266:LYS:HA	2.20	0.41
1:A:47:THR:O	1:A:52:GLY:N	2.54	0.41
1:A:28:LYS:NZ	1:A:29:THR:H	2.17	0.41
1:A:422:SER:O	1:A:423:ALA:C	2.59	0.41
1:A:256:VAL:O	1:A:266:LYS:HA	2.21	0.41
1:B:28:LYS:HA	1:B:28:LYS:HZ2	1.86	0.41
1:A:21:ARG:HD3	1:A:21:ARG:HH11	1.72	0.41
1:B:152:SER:HB3	1:B:318:ASP:HB3	2.03	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:449:SER:HB2	1:B:452:THR:HG21	2.03	0.40
1:A:432:ILE:HD12	1:B:429:GLN:HB3	2.02	0.40
1:A:124:LEU:HD23	1:A:287:ALA:HB2	2.03	0.40
1:A:110:LYS:NZ	1:A:116:SER:HB2	2.36	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	470/477 (98%)	439 (93%)	27 (6%)	4 (1%)	25	63
1	B	470/477 (98%)	436 (93%)	27 (6%)	7 (2%)	15	46
All	All	940/954 (98%)	875 (93%)	54 (6%)	11 (1%)	19	54

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	283	THR
1	B	283	THR
1	A	37	GLY
1	A	82	GLY
1	B	82	GLY
1	B	288	ALA
1	B	37	GLY
1	A	471	ILE
1	B	53	CYS
1	B	471	ILE
1	B	133	GLY

### 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	349/365 (96%)	311 (89%)	38 (11%)	9	26
1	B	349/365 (96%)	307 (88%)	42 (12%)	7	21
All	All	698/730 (96%)	618 (88%)	80 (12%)	8	23

All (80) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	VAL
1	A	21	ARG
1	A	25	LEU
1	A	28	LYS
1	A	57	LYS
1	A	79	GLU
1	A	96	ASN
1	A	101	LEU
1	A	105	ILE
1	A	107	THR
1	A	108	LEU
1	A	109	PHE
1	A	168	VAL
1	A	202	LEU
1	A	222	GLN
1	A	225	LYS
1	A	254	VAL
1	A	262	ASN
1	A	265	GLN
1	A	282	THR
1	A	283	THR
1	A	309	SER
1	A	310	VAL
1	A	319	VAL
1	A	321	ARG
1	A	330	SER
1	A	352	ILE
1	A	358	THR
1	A	368	THR
1	A	370	GLN
1	A	383	THR
1	A	391	ARG
1	A	409	LYS

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Mol	Chain	Res	Type
1	A	418	VAL
1	A	419	ILE
1	A	438	THR
1	A	462	LEU
1	A	471	ILE
1	B	6	VAL
1	B	16	TYR
1	B	21	ARG
1	B	25	LEU
1	B	28	LYS
1	B	57	LYS
1	B	73	PHE
1	B	79	GLU
1	B	88	PRO
1	B	96	ASN
1	B	101	LEU
1	B	102	THR
1	B	105	ILE
1	B	107	THR
1	B	108	LEU
1	B	156	GLU
1	B	168	VAL
1	B	202	LEU
1	B	222	GLN
1	B	225	LYS
1	B	262	ASN
1	B	265	GLN
1	B	282	THR
1	B	283	THR
1	B	309	SER
1	B	310	VAL
1	B	319	VAL
1	B	321	ARG
1	B	327	HIS
1	B	330	SER
1	B	347	MET
1	B	352	ILE
1	B	354	SER
1	B	358	THR
1	B	368	THR
1	B	370	GLN
1	B	383	THR

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Mol	Chain	Res	Type
1	B	398	THR
1	B	409	LYS
1	B	418	VAL
1	B	438	THR
1	B	462	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	120	HIS
1	A	222	GLN
1	A	262	ASN
1	A	265	GLN
1	A	346	GLN
1	A	396	ASN
1	A	417	HIS
1	A	429	GLN
1	A	458	HIS
1	B	120	HIS
1	B	222	GLN
1	B	262	ASN
1	B	346	GLN
1	B	417	HIS
1	B	429	GLN
1	B	458	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 ⓘ

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
2	FAD	A	480	-	58,58,58	1.28	4 (6%)	85,89,89	2.08	21 (24%)
2	FAD	B	480	-	58,58,58	1.43	8 (13%)	85,89,89	2.36	25 (29%)

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	480	-	-	0/34/50/50	0/1/6/6
2	FAD	B	480	-	-	0/34/50/50	0/1/6/6

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	480	FAD	C1'-C2'	6.39	1.57	1.51
2	A	480	FAD	C1'-N10	-4.87	1.42	1.48
2	B	480	FAD	C1'-N10	-3.69	1.44	1.48
2	A	480	FAD	C10-N10	-3.20	1.31	1.38
2	B	480	FAD	C4A-N9A	-3.00	1.33	1.37
2	A	480	FAD	C4A-N9A	-2.97	1.33	1.37
2	B	480	FAD	C10-N10	-2.79	1.32	1.38
2	B	480	FAD	C4-N3	2.36	1.41	1.37
2	A	480	FAD	C5A-N7A	-2.18	1.32	1.40
2	B	480	FAD	O4B-C1B	2.13	1.44	1.41
2	B	480	FAD	C9A-N10	-2.11	1.35	1.38
2	B	480	FAD	C5A-N7A	-2.01	1.32	1.40

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	480	FAD	C2-N1-C10	8.76	123.81	114.98
2	A	480	FAD	C2-N1-C10	7.46	122.49	114.98
2	B	480	FAD	N3A-C4A-N9A	6.95	137.98	125.43
2	A	480	FAD	N3A-C4A-N9A	6.70	137.53	125.43
2	B	480	FAD	N3A-C2A-N1A	-6.68	123.13	128.71
2	B	480	FAD	C4X-C10-N10	-5.53	117.75	120.51
2	B	480	FAD	C4X-C10-N1	-5.11	117.62	122.73
2	A	480	FAD	N3A-C2A-N1A	-5.11	124.44	128.71
2	B	480	FAD	C2'-C1'-N10	-4.84	106.04	112.45
2	A	480	FAD	C4X-C10-N1	-4.33	118.40	122.73
2	A	480	FAD	C6A-C5A-C4A	4.18	124.92	117.25
2	A	480	FAD	C5A-C4A-N3A	-4.13	116.71	125.70
2	B	480	FAD	O2'-C2'-C1'	4.06	119.79	109.71
2	A	480	FAD	C4X-N5-C5X	3.96	121.14	116.69
2	B	480	FAD	C4A-C5A-N7A	3.93	112.89	109.52
2	A	480	FAD	C4-N3-C2	-3.78	117.64	125.39
2	B	480	FAD	C6A-C5A-C4A	3.75	124.12	117.25
2	B	480	FAD	C4-N3-C2	-3.71	117.78	125.39
2	A	480	FAD	C4X-C10-N10	-3.61	118.71	120.51
2	B	480	FAD	C5A-C4A-N3A	-3.54	118.00	125.70
2	B	480	FAD	C9-C9A-N10	3.41	128.94	121.59
2	B	480	FAD	C4X-N5-C5X	3.34	120.45	116.69
2	B	480	FAD	N1-C10-N10	3.29	124.62	115.97
2	B	480	FAD	C4B-O4B-C1B	-3.24	106.23	109.75
2	A	480	FAD	C9-C9A-N10	3.17	128.41	121.59
2	A	480	FAD	C4A-C5A-N7A	3.15	112.22	109.52
2	A	480	FAD	O2'-C2'-C1'	3.14	117.49	109.71
2	A	480	FAD	C2'-C1'-N10	-3.08	108.36	112.45
2	B	480	FAD	C1'-N10-C9A	-2.91	116.04	118.87
2	A	480	FAD	O4B-C1B-N9A	2.80	111.04	108.44
2	B	480	FAD	C9-C9A-C5X	-2.66	114.94	119.38
2	A	480	FAD	N1-C10-N10	2.61	122.82	115.97
2	A	480	FAD	C9-C9A-C5X	-2.55	115.13	119.38
2	B	480	FAD	C9A-N10-C10	2.44	124.16	121.77
2	A	480	FAD	C6A-C5A-N7A	-2.37	122.28	131.34
2	A	480	FAD	C1'-N10-C9A	-2.36	116.57	118.87
2	A	480	FAD	C4-C4X-C10	2.32	120.69	116.95
2	A	480	FAD	P-O3P-PA	2.32	138.48	131.68
2	B	480	FAD	C1'-C2'-C3'	-2.31	103.21	109.82
2	B	480	FAD	C6A-C5A-N7A	-2.18	122.99	131.34
2	B	480	FAD	C5A-C4A-N9A	-2.18	104.02	107.16
2	B	480	FAD	C8A-N9A-C4A	2.15	108.54	106.90
2	A	480	FAD	O4B-C1B-C2B	-2.11	103.53	106.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	480	FAD	N6A-C6A-N1A	2.11	123.51	119.36
2	B	480	FAD	C2A-N1A-C6A	2.03	122.43	118.77
2	B	480	FAD	C4-C4X-C10	2.00	120.19	116.95

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	472/477 (98%)	-1.04	0	100   100	6, 26, 63, 89	0
1	B	472/477 (98%)	-0.96	2 (0%)	90   91	6, 28, 63, 90	0
All	All	944/954 (98%)	-1.00	2 (0%)	93   95	6, 27, 63, 90	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	134	LEU	3.4
1	B	262	ASN	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	A	480	53/53	0.11	0.54	9,23,30,32	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	FAD	B	480	53/53	0.10	-0.07	10,26,35,37	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.