



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 08:44 PM GMT

PDB ID : 1LVL
Title : THE REFINED STRUCTURE OF PSEUDOMONAS PUTIDA LIPOAMIDE
DEHYDROGENASE COMPLEXED WITH NAD⁺ AT 2.45 ANGSTROMS
RESOLUTION
Authors : Mattevi, A.; Hol, W.G.J.
Deposited on : 1992-12-16
Resolution : 2.45 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
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

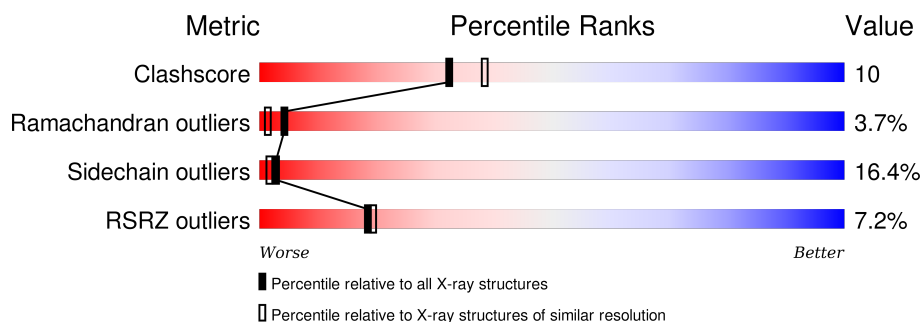
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.45 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	102246	1030 (2.48-2.44)
Ramachandran outliers	100387	1024 (2.48-2.44)
Sidechain outliers	100360	1024 (2.48-2.44)
RSRZ outliers	91569	4787 (2.50-2.42)

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. 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	458	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	FAD	A	459	X	-	-	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 3659 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 DIHYDROLIPOAMIDE DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	458	Total	C	N	O	S	0	0	0
			3372	2124	606	625	17			

- 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		

- Molecule 3 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).



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

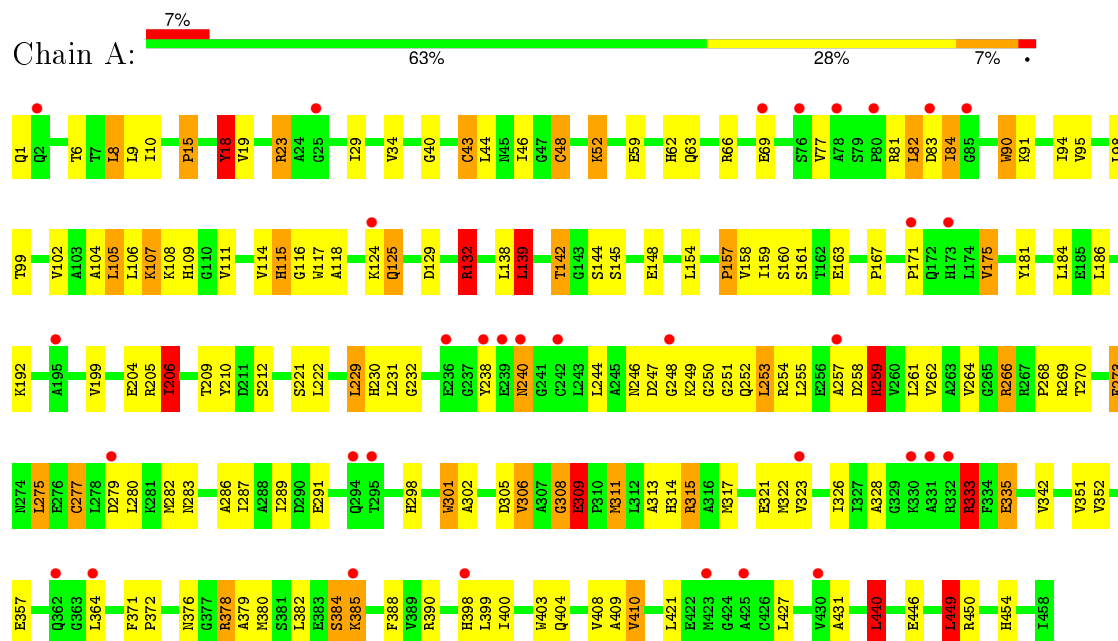
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	190	Total	O	0	0
			190	190		

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



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	64.32Å 108.12Å 151.08Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.45 12.12 – 2.45	Depositor EDS
% Data completeness (in resolution range)	(Not available) (10.00-2.45) 93.3 (12.12-2.45)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	9.06 (at 2.46Å)	Xtriage
Refinement program	GROMOS, TNT	Depositor
R, R_{free}	0.215 , (Not available) 0.259 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	44.4	Xtriage
Anisotropy	0.869	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.23 , 144.6	EDS
Estimated twinning fraction	0.010 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.029 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 18208 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	3659	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.68% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: FAD, 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	0.91	0/3428	1.73	68/4650 (1.5%)

There are no bond length outliers.

All (68) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	378	ARG	NE-CZ-NH2	-15.48	112.56	120.30
1	A	311	MET	CG-SD-CE	-11.80	81.32	100.20
1	A	333	ARG	NE-CZ-NH1	10.59	125.59	120.30
1	A	378	ARG	NE-CZ-NH1	9.29	124.94	120.30
1	A	403	TRP	CD1-CG-CD2	9.10	113.58	106.30
1	A	301	TRP	CD1-CG-CD2	8.90	113.42	106.30
1	A	23	ARG	NE-CZ-NH1	8.89	124.74	120.30
1	A	259	ARG	NE-CZ-NH1	8.82	124.71	120.30
1	A	282	MET	CA-CB-CG	-8.74	98.45	113.30
1	A	306	VAL	CA-CB-CG2	-8.42	98.27	110.90
1	A	315	ARG	NE-CZ-NH2	-8.41	116.09	120.30
1	A	450	ARG	NE-CZ-NH2	-7.69	116.46	120.30
1	A	403	TRP	CE2-CD2-CG	-7.61	101.21	107.30
1	A	301	TRP	CE2-CD2-CG	-7.41	101.37	107.30
1	A	309	GLU	CA-C-N	6.98	136.65	117.10
1	A	333	ARG	NE-CZ-NH2	-6.88	116.86	120.30
1	A	117	TRP	CE2-CD2-CG	-6.86	101.82	107.30
1	A	410	VAL	CA-CB-CG2	-6.84	100.64	110.90
1	A	90	TRP	CE2-CD2-CG	-6.78	101.88	107.30
1	A	90	TRP	CD1-CG-CD2	6.66	111.62	106.30
1	A	139	LEU	CA-CB-CG	6.63	130.54	115.30
1	A	342	VAL	CG1-CB-CG2	-6.61	100.33	110.90
1	A	317	MET	CA-CB-CG	-6.54	102.19	113.30
1	A	117	TRP	CD1-CG-CD2	6.53	111.53	106.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	66	ARG	NE-CZ-NH1	6.47	123.53	120.30
1	A	315	ARG	NE-CZ-NH1	6.34	123.47	120.30
1	A	90	TRP	CB-CG-CD1	-6.25	118.87	127.00
1	A	90	TRP	CG-CD2-CE3	6.17	139.45	133.90
1	A	77	VAL	CG1-CB-CG2	-6.11	101.13	110.90
1	A	250	GLY	CA-C-N	-6.08	104.03	116.20
1	A	81	ARG	NE-CZ-NH1	5.92	123.26	120.30
1	A	181	TYR	CA-CB-CG	5.90	124.61	113.40
1	A	238	TYR	CB-CG-CD2	-5.82	117.51	121.00
1	A	244	LEU	CA-CB-CG	5.80	128.63	115.30
1	A	66	ARG	NE-CZ-NH2	-5.70	117.45	120.30
1	A	240	ASN	CA-C-N	5.64	127.48	116.20
1	A	403	TRP	CG-CD1-NE1	-5.59	104.50	110.10
1	A	8	LEU	CA-CB-CG	5.57	128.11	115.30
1	A	175	VAL	CG1-CB-CG2	-5.55	102.03	110.90
1	A	306	VAL	CA-CB-CG1	5.55	119.22	110.90
1	A	206	ILE	N-CA-CB	-5.54	98.05	110.80
1	A	148	GLU	CA-CB-CG	-5.52	101.25	113.40
1	A	308	GLY	O-C-N	5.45	131.42	122.70
1	A	301	TRP	CG-CD1-NE1	-5.45	104.65	110.10
1	A	309	GLU	CA-C-O	-5.33	108.90	120.10
1	A	158	VAL	N-CA-C	-5.33	96.62	111.00
1	A	48	CYS	CA-CB-SG	-5.32	104.42	114.00
1	A	449	LEU	CB-CG-CD2	-5.32	101.96	111.00
1	A	273	PHE	N-CA-C	-5.30	96.68	111.00
1	A	390	ARG	NE-CZ-NH1	5.29	122.95	120.30
1	A	454	HIS	N-CA-C	5.22	125.11	111.00
1	A	323	VAL	CA-CB-CG2	-5.22	103.07	110.90
1	A	277	CYS	CA-CB-SG	-5.21	104.63	114.00
1	A	266	ARG	NE-CZ-NH2	-5.19	117.71	120.30
1	A	357	GLU	CA-CB-CG	5.18	124.81	113.40
1	A	18	TYR	CA-CB-CG	5.18	123.25	113.40
1	A	83	ASP	N-CA-C	-5.14	97.11	111.00
1	A	410	VAL	CA-CB-CG1	5.14	118.61	110.90
1	A	23	ARG	NE-CZ-NH2	-5.07	117.76	120.30
1	A	186	LEU	CB-CG-CD2	-5.07	102.39	111.00
1	A	380	MET	CG-SD-CE	-5.07	92.09	100.20
1	A	259	ARG	NE-CZ-NH2	-5.05	117.78	120.30
1	A	117	TRP	CA-CB-CG	-5.04	104.12	113.70
1	A	440	LEU	O-C-N	-5.03	114.65	123.20
1	A	125	GLN	CA-CB-CG	5.02	124.45	113.40
1	A	132	ARG	NE-CZ-NH1	5.02	122.81	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	308	GLY	CA-C-N	-5.01	106.17	117.20
1	A	385	LYS	CA-C-N	-5.01	106.18	117.20

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	3372	0	3449	72	0
2	A	53	0	31	2	0
3	A	44	0	26	6	0
4	A	190	0	0	2	2
All	All	3659	0	3506	73	2

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 10.

All (73) 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)
3:A:460:NAD:O5D	3:A:460:NAD:C5D	1.72	1.36
1:A:376:ASN:HD22	1:A:379:ALA:H	1.25	0.81
1:A:376:ASN:ND2	1:A:379:ALA:H	1.80	0.80
1:A:142:THR:HG22	2:A:459:FAD:N7A	2.00	0.78
1:A:431:ALA:HB1	1:A:449:LEU:HD13	1.69	0.74
1:A:15:PRO:HD3	1:A:40:GLY:O	1.87	0.73
1:A:144:SER:HB2	1:A:305:ASP:HB3	1.70	0.72
1:A:171:PRO:HB3	1:A:259:ARG:HG3	1.74	0.70
1:A:175:VAL:HG23	1:A:257:ALA:HB2	1.73	0.70
1:A:206:ILE:HG12	1:A:229:LEU:HD21	1.74	0.70
1:A:159:ILE:HB	1:A:163:GLU:HB2	1.74	0.69
1:A:125:GLN:OE1	1:A:132:ARG:HB3	1.94	0.67
1:A:376:ASN:HD21	1:A:378:ARG:HB3	1.60	0.67
1:A:266:ARG:HG3	3:A:460:NAD:H52N	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:376:ASN:HD22	1:A:379:ALA:N	1.95	0.64
1:A:311:MET:HB2	3:A:460:NAD:H2D	1.81	0.63
1:A:351:VAL:HG13	1:A:404:GLN:HG3	1.78	0.63
1:A:291:GLU:HG3	1:A:333:ARG:HG3	1.83	0.61
1:A:258:ASP:O	1:A:259:ARG:HG2	2.01	0.60
1:A:98:LEU:O	1:A:102:VAL:HG23	2.04	0.57
1:A:205:ARG:HA	1:A:231:LEU:HD13	1.86	0.57
1:A:52:LYS:N	1:A:52:LYS:HD3	2.19	0.56
1:A:62:HIS:HB2	1:A:192:LYS:HB3	1.87	0.56
1:A:199:VAL:HG11	1:A:206:ILE:HD11	1.88	0.56
1:A:268:PRO:HG2	1:A:286:ALA:HB2	1.88	0.55
1:A:266:ARG:HG3	3:A:460:NAD:C5D	2.36	0.55
1:A:204:GLU:O	1:A:231:LEU:HD13	2.07	0.55
1:A:139:LEU:HD23	1:A:301:TRP:HB2	1.90	0.53
1:A:184:LEU:HD11	1:A:206:ILE:HG23	1.90	0.53
1:A:206:ILE:CG1	1:A:229:LEU:HD21	2.39	0.53
1:A:142:THR:HG21	1:A:273:PHE:CZ	2.44	0.52
1:A:398:HIS:ND1	1:A:427:LEU:HD12	2.25	0.52
1:A:154:LEU:HD21	1:A:160:SER:HB3	1.93	0.51
1:A:29:ILE:HD11	1:A:328:ALA:HB2	1.93	0.50
1:A:270:THR:HG23	1:A:275:LEU:HD13	1.94	0.50
1:A:10:ILE:HG12	1:A:139:LEU:HD12	1.94	0.50
1:A:247:ASP:OD2	1:A:251:GLY:HA3	2.13	0.49
1:A:34:VAL:HG11	1:A:118:ALA:HB2	1.95	0.49
1:A:400:ILE:HD11	1:A:427:LEU:HA	1.95	0.49
1:A:230:HIS:CD2	1:A:253:LEU:HD11	2.48	0.49
1:A:105:LEU:O	1:A:109:HIS:HD2	1.95	0.48
1:A:18:TYR:CD1	1:A:19:VAL:HG23	2.49	0.48
1:A:322:MET:O	1:A:326:ILE:HG13	2.15	0.47
1:A:18:TYR:HE2	1:A:40:GLY:HA2	1.80	0.47
1:A:82:LEU:HD21	1:A:84:ILE:HG23	1.97	0.46
1:A:372:PRO:HA	1:A:388:PHE:HA	1.98	0.46
1:A:175:VAL:HG23	1:A:257:ALA:CB	2.44	0.46
1:A:90:TRP:CZ2	1:A:94:ILE:HD11	2.51	0.46
1:A:333:ARG:CZ	1:A:335:GLU:HG2	2.47	0.45
1:A:43:CYS:SG	1:A:313:ALA:HB2	2.57	0.45
1:A:175:VAL:CG2	1:A:257:ALA:HB2	2.43	0.45
1:A:104:ALA:O	1:A:108:LYS:HB2	2.17	0.45
1:A:44:LEU:O	1:A:95:VAL:HG13	2.15	0.45
1:A:289:ILE:CG2	1:A:302:ALA:HB3	2.47	0.45
1:A:205:ARG:HA	1:A:231:LEU:CD1	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:352:VAL:HG12	1:A:421:LEU:HD12	1.99	0.44
1:A:273:PHE:CZ	1:A:275:LEU:HD12	2.53	0.44
1:A:91:LYS:O	1:A:95:VAL:HG23	2.18	0.44
1:A:364:LEU:HD11	4:A:555:HOH:O	2.18	0.43
1:A:289:ILE:HG21	1:A:302:ALA:HB3	2.00	0.43
1:A:378:ARG:HG3	1:A:440:LEU:HD13	2.00	0.43
1:A:210:TYR:CE1	1:A:351:VAL:HG21	2.53	0.43
1:A:371:PHE:CD2	1:A:446:GLU:HB3	2.53	0.43
1:A:107:LYS:HE2	1:A:107:LYS:HA	2.00	0.43
1:A:311:MET:CB	3:A:460:NAD:H2D	2.47	0.42
1:A:138:LEU:O	1:A:301:TRP:HD1	2.03	0.42
1:A:313:ALA:N	2:A:459:FAD:O3'	2.54	0.41
1:A:230:HIS:HE1	4:A:474:HOH:O	2.03	0.41
1:A:309:GLU:HB2	1:A:315:ARG:NH2	2.35	0.41
1:A:275:LEU:HD11	1:A:287:ILE:HD11	2.03	0.41
1:A:262:VAL:HG12	1:A:264:VAL:HG22	2.03	0.40
1:A:311:MET:H	3:A:460:NAD:C5N	2.33	0.40
1:A:59:GLU:O	1:A:63:GLN:HG2	2.22	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:477:HOH:O	4:A:644:HOH:O[5_455]	1.70	0.50
4:A:530:HOH:O	4:A:543:HOH:O[5_555]	1.90	0.30

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	456/458 (100%)	402 (88%)	37 (8%)	17 (4%)	4 1

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	124	LYS
1	A	157	PRO
1	A	248	GLY
1	A	253	LEU
1	A	298	HIS
1	A	309	GLU
1	A	48	CYS
1	A	240	ASN
1	A	384	SER
1	A	279	ASP
1	A	385	LYS
1	A	409	ALA
1	A	115	HIS
1	A	232	GLY
1	A	46	ILE
1	A	116	GLY
1	A	308	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	348/348 (100%)	291 (84%)	57 (16%)	3 2

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	GLN
1	A	6	THR
1	A	8	LEU
1	A	9	LEU
1	A	15	PRO
1	A	18	TYR
1	A	23	ARG
1	A	43	CYS

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Mol	Chain	Res	Type
1	A	52	LYS
1	A	69	GLU
1	A	82	LEU
1	A	84	ILE
1	A	99	THR
1	A	105	LEU
1	A	106	LEU
1	A	107	LYS
1	A	111	VAL
1	A	114	VAL
1	A	115	HIS
1	A	129	ASP
1	A	132	ARG
1	A	139	LEU
1	A	142	THR
1	A	145	SER
1	A	157	PRO
1	A	161	SER
1	A	167	PRO
1	A	206	ILE
1	A	209	THR
1	A	212	SER
1	A	221	SER
1	A	222	LEU
1	A	229	LEU
1	A	246	ASN
1	A	249	LYS
1	A	252	GLN
1	A	254	ARG
1	A	255	LEU
1	A	259	ARG
1	A	261	LEU
1	A	269	ARG
1	A	275	LEU
1	A	277	CYS
1	A	280	LEU
1	A	283	ASN
1	A	306	VAL
1	A	314	HIS
1	A	321	GLU
1	A	333	ARG
1	A	335	GLU

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Mol	Chain	Res	Type
1	A	382	LEU
1	A	384	SER
1	A	399	LEU
1	A	408	VAL
1	A	410	VAL
1	A	440	LEU
1	A	449	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	109	HIS
1	A	137	HIS
1	A	230	HIS
1	A	376	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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	459	-	48,58,58	1.32	7 (14%)	54,89,89	2.50	13 (24%)
3	NAD	A	460	-	38,48,48	1.61	6 (15%)	47,73,73	1.55	6 (12%)

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	459	-	1/1/9/9	0/30/50/50	0/6/6/6
3	NAD	A	460	-	-	0/22/62/62	0/5/5/5

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	459	FAD	C1'-N10	-2.53	1.45	1.48
2	A	459	FAD	O5'-C5'	-2.53	1.34	1.44
2	A	459	FAD	C6-C5X	-2.52	1.37	1.41
2	A	459	FAD	C9A-C5X	-2.24	1.38	1.42
2	A	459	FAD	C4'-C3'	-2.23	1.48	1.53
3	A	460	NAD	C5A-N7A	-2.03	1.32	1.39
3	A	460	NAD	C6N-N1N	2.21	1.41	1.35
2	A	459	FAD	O4B-C1B	2.48	1.44	1.41
3	A	460	NAD	C3N-C7N	2.84	1.55	1.50
3	A	460	NAD	O4B-C1B	3.26	1.45	1.41
3	A	460	NAD	O4D-C1D	3.35	1.45	1.41
2	A	459	FAD	C4-N3	4.06	1.40	1.33
3	A	460	NAD	O5D-C5D	6.73	1.72	1.44

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	459	FAD	C4X-C10-N10	-6.28	116.82	120.52
3	A	460	NAD	N3A-C2A-N1A	-6.19	124.15	128.89
2	A	459	FAD	N3A-C2A-N1A	-6.16	124.18	128.89
2	A	459	FAD	C4X-C4-N3	-4.57	117.34	123.59
2	A	459	FAD	C4B-O4B-C1B	-3.58	105.78	109.72
3	A	460	NAD	C4D-O4D-C1D	-3.27	106.13	109.72
2	A	459	FAD	C4-C4X-C10	-2.98	118.03	119.94
2	A	459	FAD	O5B-PA-O1A	-2.74	98.97	109.62
3	A	460	NAD	O3-PA-O5B	-2.50	96.32	102.94
2	A	459	FAD	O3P-P-O5'	-2.19	97.12	102.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	460	NAD	O4B-C1B-N9A	2.11	112.52	108.10
2	A	459	FAD	O4'-C4'-C5'	2.23	115.05	110.19
3	A	460	NAD	O4D-C1D-N1N	2.30	110.66	108.13
2	A	459	FAD	P-O3P-PA	3.12	141.49	132.73
2	A	459	FAD	C4X-N5-C5X	3.19	120.43	116.76
2	A	459	FAD	C4A-C5A-N7A	3.25	112.47	109.48
3	A	460	NAD	C4A-C5A-N7A	3.26	112.48	109.48
2	A	459	FAD	C4-N3-C2	7.61	121.83	115.25
2	A	459	FAD	C1'-N10-C9A	8.94	128.90	118.86

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	459	FAD	C2'

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	459	FAD	2	0
3	A	460	NAD	6	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

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	458/458 (100%)	0.29	33 (7%)	18 19	11, 38, 77, 90	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	398	HIS	5.0
1	A	330	LYS	4.9
1	A	248	GLY	3.6
1	A	80	PRO	3.6
1	A	364	LEU	3.5
1	A	195	ALA	3.3
1	A	124	LYS	3.2
1	A	257	ALA	3.2
1	A	331	ALA	3.2
1	A	69	GLU	3.1
1	A	430	VAL	3.0
1	A	323	VAL	2.8
1	A	242	CYS	2.8
1	A	2	GLN	2.7
1	A	240	ASN	2.7
1	A	78	ALA	2.7
1	A	171	PRO	2.6
1	A	173	HIS	2.4
1	A	294	GLN	2.3
1	A	85	GLY	2.3
1	A	425	ALA	2.3
1	A	423	MET	2.3
1	A	83	ASP	2.3
1	A	76	SER	2.3
1	A	239	GLU	2.2
1	A	25	GLY	2.2
1	A	332	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	238	TYR	2.2
1	A	362	GLN	2.1
1	A	279	ASP	2.1
1	A	295	THR	2.1
1	A	385	LYS	2.1
1	A	236	GLU	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, 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	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	NAD	A	460	44/44	0.90	0.18	0.69	55,72,90,90	0
2	FAD	A	459	53/53	0.94	0.15	0.52	4,27,62,68	0

6.5 Other polymers [i](#)

There are no such residues in this entry.