



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 05:42 AM UTC

PDB ID : 1LVL / pdb_00001lvl
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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

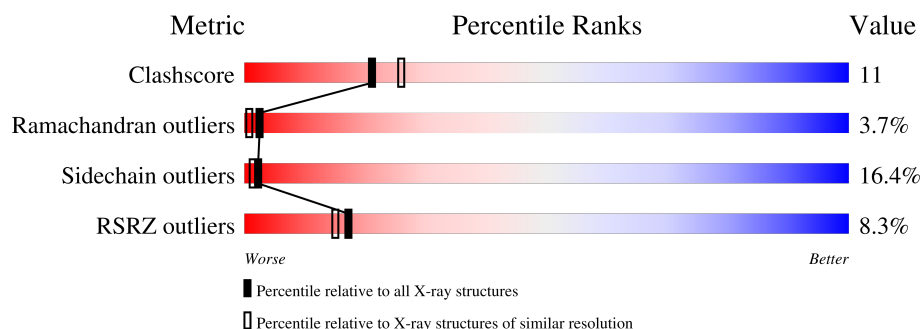
1 Overall quality at a glance

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	190562	1229 (2.46-2.46)
Ramachandran outliers	187476	1218 (2.46-2.46)
Sidechain outliers	187428	1218 (2.46-2.46)
RSRZ outliers	180081	1190 (2.46-2.46)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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](#)

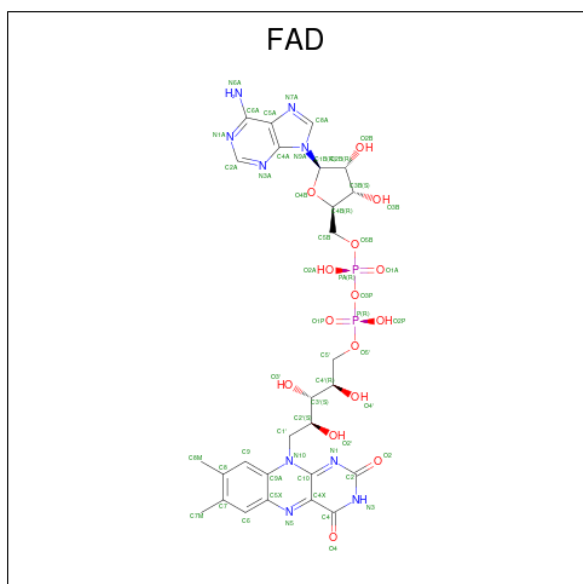
There are 4 unique types of molecules in this entry. The entry contains 3659 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

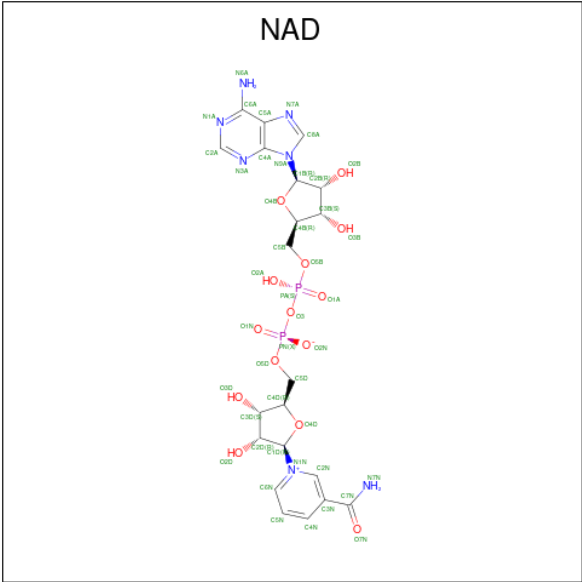
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	458	3372	2124	606	625	17	0	0	0

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



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

- Molecule 3 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: 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		

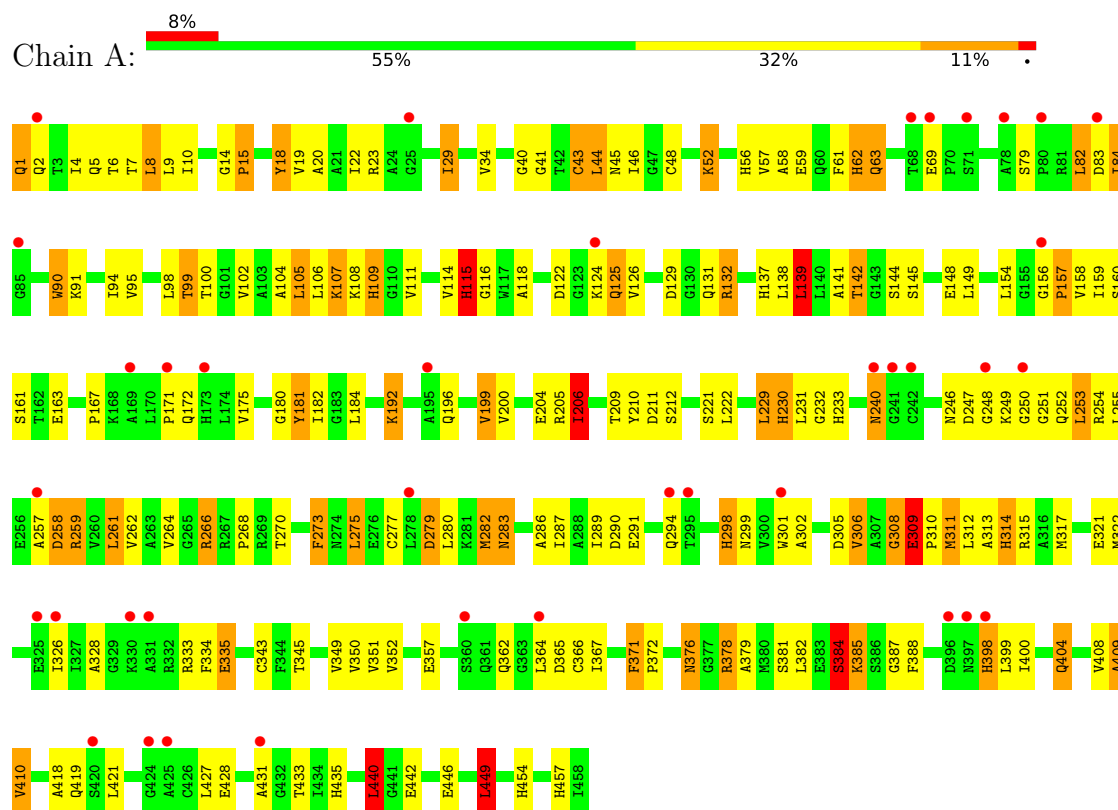
- Molecule 4 is water.

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, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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 10.00 – 2.45	Depositor EDS
% Data completeness (in resolution range)	(Not available) (10.00-2.45) 91.6 (10.00-2.45)	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) 0.257 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	44.4	Xtriage
Anisotropy	0.869	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.13 , 94.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
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
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, 0.333 respectively for untwinned datasets, and 0.375, 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: NAD, 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	1.22	23/3428 (0.7%)	2.06	125/4650 (2.7%)

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	109	HIS	CD2-NE2	-6.83	1.30	1.37
1	A	398	HIS	CD2-NE2	-6.51	1.30	1.37
1	A	62	HIS	CD2-NE2	-6.32	1.30	1.37
1	A	182	ILE	CA-CB	6.25	1.61	1.54
1	A	115	HIS	CD2-NE2	-6.25	1.30	1.37
1	A	233	HIS	CD2-NE2	-6.16	1.31	1.37
1	A	44	LEU	CA-C	-5.73	1.44	1.52
1	A	454	HIS	CG-ND1	-5.50	1.32	1.38
1	A	109	HIS	CG-ND1	-5.50	1.32	1.38
1	A	398	HIS	CG-ND1	-5.47	1.32	1.38
1	A	343	CYS	CA-CB	5.40	1.61	1.53
1	A	298	HIS	CD2-NE2	-5.38	1.31	1.37
1	A	62	HIS	CG-ND1	-5.32	1.32	1.38
1	A	435	HIS	CG-ND1	-5.24	1.32	1.38
1	A	230	HIS	CD2-NE2	-5.22	1.32	1.37
1	A	230	HIS	CG-ND1	-5.21	1.32	1.38
1	A	454	HIS	CD2-NE2	-5.21	1.32	1.37
1	A	457	HIS	CD2-NE2	-5.21	1.32	1.37
1	A	298	HIS	CG-ND1	-5.19	1.32	1.38
1	A	115	HIS	CG-ND1	-5.15	1.32	1.38
1	A	56	HIS	CD2-NE2	-5.14	1.32	1.37
1	A	435	HIS	CD2-NE2	-5.05	1.32	1.37
1	A	137	HIS	CG-ND1	-5.05	1.32	1.38

All (125) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	62	HIS	ND1-CG-CD2	9.56	115.66	106.10
1	A	211	ASP	CA-CB-CG	9.52	122.12	112.60
1	A	376	ASN	OD1-CG-ND2	-9.42	113.18	122.60
1	A	299	ASN	OD1-CG-ND2	-9.05	113.55	122.60
1	A	311	MET	CG-SD-CE	-8.90	81.32	100.90
1	A	454	HIS	ND1-CG-CD2	8.79	114.89	106.10
1	A	115	HIS	ND1-CG-CD2	8.44	114.54	106.10
1	A	279	ASP	CA-CB-CG	8.30	120.90	112.60
1	A	309	GLU	CA-C-O	-8.22	108.90	120.16
1	A	273	PHE	N-CA-C	-8.11	96.68	109.50
1	A	283	ASN	CA-CB-CG	8.03	120.63	112.60
1	A	457	HIS	ND1-CG-CD2	8.02	114.12	106.10
1	A	454	HIS	N-CA-C	8.01	125.11	108.53
1	A	206	ILE	N-CA-CB	-7.99	98.05	111.23
1	A	290	ASP	CA-CB-CG	7.91	120.51	112.60
1	A	230	HIS	ND1-CG-CD2	7.83	113.94	106.10
1	A	282	MET	CA-CB-CG	-7.83	98.45	114.10
1	A	294	GLN	OE1-CD-NE2	-7.81	114.79	122.60
1	A	158	VAL	N-CA-C	-7.71	96.62	107.80
1	A	109	HIS	ND1-CG-CD2	7.58	113.68	106.10
1	A	334	PHE	CA-CB-CG	7.55	121.35	113.80
1	A	56	HIS	ND1-CG-CD2	7.43	113.53	106.10
1	A	378	ARG	NE-CZ-NH2	-7.38	112.56	119.20
1	A	141	ALA	CA-C-O	7.34	128.50	121.67
1	A	433	THR	N-CA-C	-7.21	97.64	109.40
1	A	306	VAL	CA-CB-CG2	-7.14	98.27	110.40
1	A	196	GLN	OE1-CD-NE2	-7.09	115.51	122.60
1	A	314	HIS	CG-CD2-NE2	-7.07	100.14	107.20
1	A	314	HIS	ND1-CG-CD2	7.00	113.10	106.10
1	A	181	TYR	N-CA-C	6.93	118.83	111.28
1	A	404	GLN	OE1-CD-NE2	-6.91	115.69	122.60
1	A	299	ASN	CB-CG-ND2	6.86	126.69	116.40
1	A	4	ILE	N-CA-C	-6.85	99.89	109.21
1	A	125	GLN	OE1-CD-NE2	-6.85	115.75	122.60
1	A	196	GLN	CG-CD-NE2	6.83	126.64	116.40
1	A	367	ILE	N-CA-C	-6.80	98.63	108.36
1	A	311	MET	N-CA-C	6.75	120.86	108.58
1	A	308	GLY	O-C-N	6.71	131.42	122.70
1	A	381	SER	CA-CB-OG	6.58	124.25	111.10
1	A	62	HIS	CG-CD2-NE2	-6.57	100.63	107.20
1	A	371	PHE	CA-C-N	6.57	126.75	120.31
1	A	371	PHE	C-N-CA	6.57	126.75	120.31
1	A	20	ALA	N-CA-C	-6.52	104.25	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	230	HIS	CA-CB-CG	-6.52	107.28	113.80
1	A	350	VAL	N-CA-C	-6.52	99.34	108.27
1	A	273	PHE	CA-CB-CG	6.49	120.29	113.80
1	A	115	HIS	CG-CD2-NE2	-6.47	100.73	107.20
1	A	310	PRO	N-CA-CB	6.47	106.54	102.92
1	A	156	GLY	CA-C-N	6.46	127.92	119.84
1	A	156	GLY	C-N-CA	6.46	127.92	119.84
1	A	148	GLU	CA-CB-CG	-6.42	101.25	114.10
1	A	457	HIS	CG-CD2-NE2	-6.40	100.80	107.20
1	A	384	SER	N-CA-C	6.37	124.36	110.80
1	A	122	ASP	CA-CB-CG	6.35	118.95	112.60
1	A	230	HIS	CG-CD2-NE2	-6.30	100.90	107.20
1	A	83	ASP	N-CA-C	-6.23	97.11	108.02
1	A	365	ASP	CA-CB-CG	6.14	118.74	112.60
1	A	309	GLU	O-C-N	-5.98	114.44	121.32
1	A	233	HIS	ND1-CG-CD2	5.96	112.06	106.10
1	A	317	MET	CA-CB-CG	-5.96	102.19	114.10
1	A	181	TYR	CA-CB-CG	5.95	124.61	113.90
1	A	440	LEU	O-C-N	-5.91	114.65	122.33
1	A	99	THR	N-CA-C	-5.87	104.80	111.14
1	A	298	HIS	ND1-CG-CD2	5.85	111.95	106.10
1	A	56	HIS	CG-CD2-NE2	-5.84	101.36	107.20
1	A	250	GLY	O-C-N	5.82	130.27	122.70
1	A	100	THR	CA-CB-OG1	-5.78	100.93	109.60
1	A	398	HIS	ND1-CG-CD2	5.76	111.86	106.10
1	A	4	ILE	O-C-N	-5.75	115.94	122.72
1	A	410	VAL	CA-CB-CG2	-5.74	100.64	110.40
1	A	240	ASN	OD1-CG-ND2	-5.74	116.86	122.60
1	A	61	PHE	CA-CB-CG	-5.74	108.06	113.80
1	A	233	HIS	CB-CG-CD2	-5.68	123.81	131.20
1	A	137	HIS	ND1-CG-CD2	5.65	111.75	106.10
1	A	149	LEU	CA-C-N	5.63	124.83	118.97
1	A	149	LEU	C-N-CA	5.63	124.83	118.97
1	A	454	HIS	CB-CG-CD2	-5.61	123.91	131.20
1	A	1	GLN	OE1-CD-NE2	-5.59	117.01	122.60
1	A	428	GLU	N-CA-C	5.58	117.36	111.28
1	A	266	ARG	CA-CB-CG	-5.58	102.94	114.10
1	A	449	LEU	N-CA-C	-5.58	104.83	111.69
1	A	22	ILE	CA-C-O	-5.57	113.82	120.78
1	A	90	TRP	CG-CD2-CE3	5.55	139.45	133.90
1	A	442	GLU	N-CA-C	-5.51	105.35	111.36
1	A	454	HIS	CG-CD2-NE2	-5.47	101.73	107.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	139	LEU	N-CA-C	-5.46	99.53	108.76
1	A	385	LYS	CA-C-O	5.43	128.27	120.51
1	A	7	THR	N-CA-C	-5.42	105.47	112.68
1	A	366	CYS	N-CA-C	5.42	118.39	109.72
1	A	62	HIS	CB-CG-CD2	-5.40	124.18	131.20
1	A	5	GLN	OE1-CD-NE2	-5.38	117.22	122.60
1	A	282	MET	N-CA-C	5.38	118.03	109.81
1	A	90	TRP	CB-CG-CD1	-5.35	118.87	126.90
1	A	357	GLU	CA-CB-CG	5.35	124.81	114.10
1	A	63	GLN	OE1-CD-NE2	-5.34	117.26	122.60
1	A	409	ALA	N-CA-C	5.33	122.15	110.80
1	A	199	VAL	N-CA-C	-5.33	100.71	108.17
1	A	79	SER	N-CA-C	5.31	123.39	112.40
1	A	192	LYS	CG-CD-CE	-5.30	99.10	111.30
1	A	418	ALA	N-CA-C	5.29	116.73	111.07
1	A	45	ASN	N-CA-C	5.27	119.80	112.90
1	A	349	VAL	N-CA-C	-5.25	100.77	108.85
1	A	261	LEU	N-CA-C	-5.24	98.73	107.80
1	A	314	HIS	CE1-NE2-CD2	5.24	114.24	109.00
1	A	58	ALA	N-CA-C	-5.23	105.50	111.14
1	A	2	GLN	N-CA-C	5.21	118.22	110.14
1	A	29	ILE	N-CA-C	-5.21	101.90	108.05
1	A	8	LEU	O-C-N	5.21	129.31	123.27
1	A	387	GLY	N-CA-C	-5.20	100.86	113.18
1	A	18	TYR	CA-CB-CG	5.19	123.25	113.90
1	A	306	VAL	CA-CB-CG1	5.19	119.22	110.40
1	A	200	VAL	N-CA-C	-5.18	100.85	108.11
1	A	125	GLN	CA-CB-CG	5.17	124.45	114.10
1	A	132	ARG	N-CA-C	-5.17	103.57	110.55
1	A	172	GLN	OE1-CD-NE2	-5.13	117.47	122.60
1	A	362	GLN	OE1-CD-NE2	-5.12	117.48	122.60
1	A	457	HIS	CB-CG-CD2	-5.12	124.55	131.20
1	A	419	GLN	OE1-CD-NE2	-5.11	117.49	122.60
1	A	131	GLN	CA-CB-CG	5.10	124.29	114.10
1	A	14	GLY	CA-C-N	5.08	126.20	119.84
1	A	14	GLY	C-N-CA	5.08	126.20	119.84
1	A	206	ILE	CB-CA-C	5.07	119.61	111.29
1	A	41	GLY	O-C-N	5.06	127.25	122.90
1	A	258	ASP	CA-CB-CG	5.05	117.65	112.60
1	A	180	GLY	CA-C-O	-5.02	115.76	122.23

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	76	0
2	A	53	0	31	2	0
3	A	44	0	26	7	0
4	A	190	0	0	2	2
All	All	3659	0	3506	77	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 11.

All (77) 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
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:270:THR:HG21	1:A:282:MET:HE1	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:98:LEU:O	1:A:102:VAL:HG23	2.04	0.57
1:A:181:TYR:HH	3:A:460:NAD:HO2N	1.53	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:90:TRP:CZ2	1:A:94:ILE:HD11	2.51	0.46
1:A:175:VAL:HG23	1:A:257:ALA:CB	2.44	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:104:ALA:O	1:A:108:LYS:HB2	2.17	0.45
1:A:175:VAL:CG2	1:A:257:ALA:HB2	2.43	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
1:A:247:ASP:CG	1:A:251:GLY:HA3	2.41	0.44
1:A:352:VAL:HG12	1:A:421:LEU:HD12	1.99	0.44
1:A:91:LYS:O	1:A:95:VAL:HG23	2.18	0.44
1:A:273:PHE:CZ	1:A:275:LEU:HD12	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:322:MET:HE2	1:A:322:MET:HB3	1.83	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:HA	1:A:107:LYS:HE2	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%)	2 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%)	2 1

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	23	ARG
1	A	43	CYS
1	A	52	LYS
1	A	57	VAL
1	A	69	GLU

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Mol	Chain	Res	Type
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	126	VAL
1	A	129	ASP
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	275	LEU
1	A	277	CYS
1	A	280	LEU
1	A	283	ASN
1	A	306	VAL
1	A	312	LEU
1	A	314	HIS
1	A	321	GLU
1	A	335	GLU
1	A	345	THR
1	A	382	LEU
1	A	384	SER

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	GLN
1	A	109	HIS
1	A	137	HIS
1	A	172	GLN
1	A	230	HIS
1	A	252	GLN
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 oligosaccharides 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	-	58,58,58	1.32	6 (10%)	85,89,89	1.91	18 (21%)
3	NAD	A	460	-	46,48,48	1.83	7 (15%)	64,73,73	2.04	12 (18%)

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	16/34/50/50	0/6/6/6
3	NAD	A	460	-	-	6/30/62/62	0/5/5/5

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	460	NAD	O5D-C5D	7.32	1.72	1.44
3	A	460	NAD	C2N-N1N	5.29	1.40	1.35
2	A	459	FAD	C1'-C2'	-3.60	1.47	1.52
3	A	460	NAD	C5A-N7A	-3.59	1.32	1.39
2	A	459	FAD	C5A-N7A	-3.53	1.32	1.39
3	A	460	NAD	O4D-C1D	3.46	1.45	1.40
3	A	460	NAD	C3N-C7N	2.96	1.55	1.50
2	A	459	FAD	O5'-C5'	-2.68	1.34	1.44
3	A	460	NAD	C6N-N1N	2.66	1.41	1.35
2	A	459	FAD	C4'-C3'	-2.58	1.48	1.53
2	A	459	FAD	C5X-N5	-2.42	1.35	1.39
3	A	460	NAD	PN-O3	2.29	1.62	1.59
2	A	459	FAD	C2-N1	-2.09	1.31	1.36

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	460	NAD	C5A-C4A-N3A	-7.54	116.34	126.72
2	A	459	FAD	C5A-C4A-N3A	-7.09	116.96	126.72
3	A	460	NAD	N3A-C4A-N9A	6.60	138.39	127.17
2	A	459	FAD	N3A-C4A-N9A	6.41	138.07	127.17
2	A	459	FAD	C6A-C5A-C4A	5.19	124.27	117.18
3	A	460	NAD	C6A-C5A-C4A	5.12	124.17	117.18
2	A	459	FAD	C6A-C5A-N7A	-4.83	122.77	132.09
3	A	460	NAD	C6A-C5A-N7A	-4.56	123.30	132.09
2	A	459	FAD	C1'-N10-C9A	4.25	128.90	120.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	460	NAD	C4D-O4D-C1D	-4.15	106.13	109.92
2	A	459	FAD	C5'-C4'-C3'	-3.91	104.84	112.22
3	A	460	NAD	C6N-N1N-C2N	-3.77	118.67	121.88
2	A	459	FAD	O4-C4-C4X	-3.29	117.84	126.53
3	A	460	NAD	C2A-N3A-C4A	3.16	119.55	111.83
3	A	460	NAD	PN-O5D-C5D	3.00	138.56	121.35
3	A	460	NAD	N3A-C2A-N1A	-2.93	124.15	128.58
2	A	459	FAD	N3A-C2A-N1A	-2.91	124.18	128.58
2	A	459	FAD	C2A-N3A-C4A	2.79	118.64	111.83
2	A	459	FAD	C2'-C1'-N10	2.74	123.16	110.20
2	A	459	FAD	O5B-PA-O1A	-2.51	98.97	108.94
2	A	459	FAD	O4-C4-N3	2.47	124.76	120.11
2	A	459	FAD	C4'-C3'-C2'	2.46	117.66	113.57
3	A	460	NAD	O4B-C1B-N9A	2.31	112.52	108.09
2	A	459	FAD	O4'-C4'-C5'	2.29	115.05	109.99
3	A	460	NAD	O4B-C4B-C5B	2.23	116.47	109.33
2	A	459	FAD	C4-N3-C2	-2.15	121.83	125.64
2	A	459	FAD	O5'-C5'-C4'	2.10	114.96	109.36
2	A	459	FAD	N6A-C6A-N1A	2.06	122.95	118.38
2	A	459	FAD	C4A-N9A-C8A	2.05	107.89	105.74
3	A	460	NAD	O2B-C2B-C1B	2.02	117.06	110.10

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	459	FAD	C2'

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	459	FAD	C2'-C1'-N10-C9A
2	A	459	FAD	C2'-C1'-N10-C10
2	A	459	FAD	N10-C1'-C2'-O2'
2	A	459	FAD	C1'-C2'-C3'-O3'
2	A	459	FAD	C1'-C2'-C3'-C4'
2	A	459	FAD	O2'-C2'-C3'-O3'
2	A	459	FAD	O2'-C2'-C3'-C4'
2	A	459	FAD	C5'-O5'-P-O1P
2	A	459	FAD	C5'-O5'-P-O2P
2	A	459	FAD	C5'-O5'-P-O3P
3	A	460	NAD	C5B-O5B-PA-O2A
3	A	460	NAD	C5B-O5B-PA-O3

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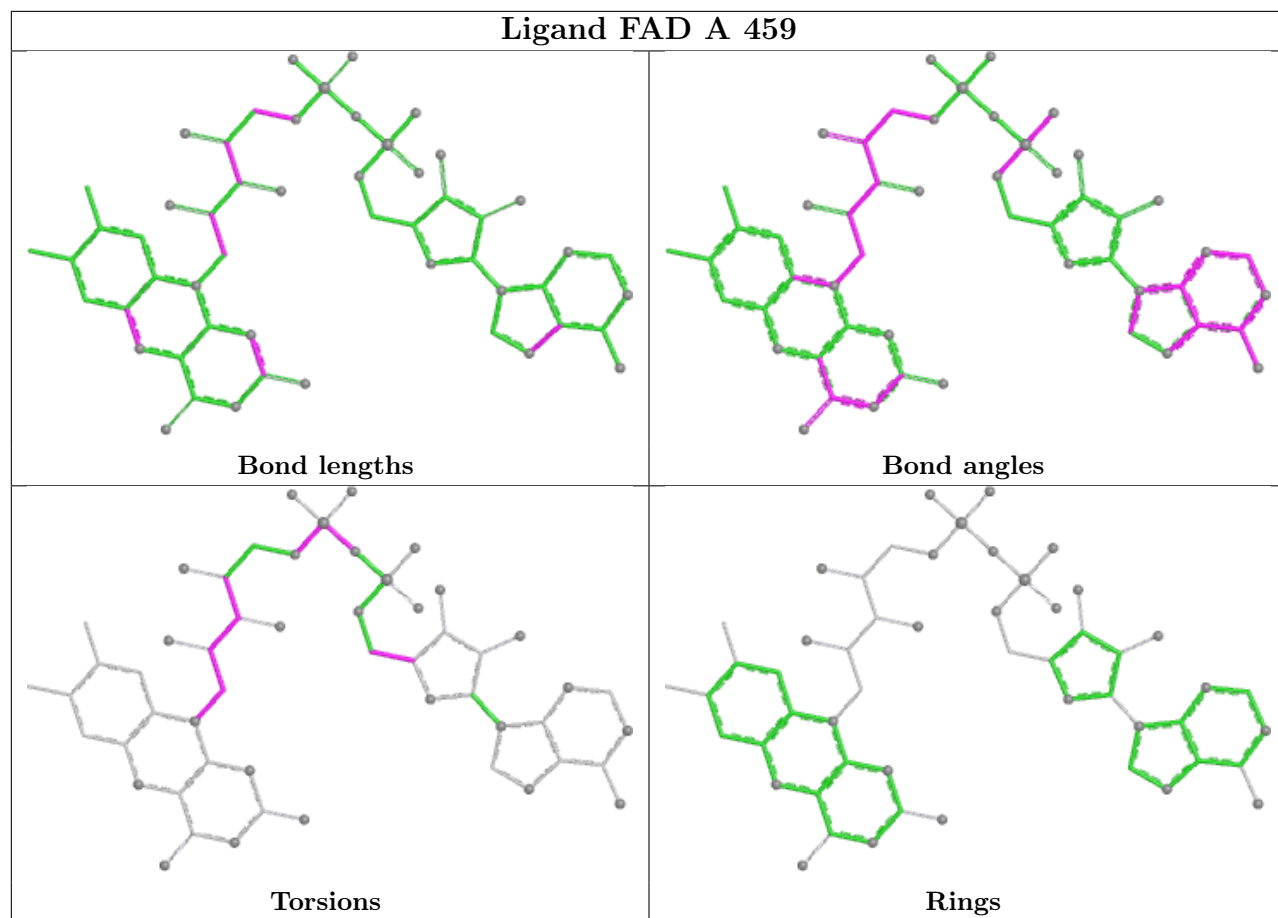
Mol	Chain	Res	Type	Atoms
3	A	460	NAD	PN-O3-PA-O5B
3	A	460	NAD	C4D-C5D-O5D-PN
2	A	459	FAD	C2'-C3'-C4'-O4'
2	A	459	FAD	C2'-C3'-C4'-C5'
2	A	459	FAD	O3'-C3'-C4'-O4'
2	A	459	FAD	PA-O3P-P-O5'
2	A	459	FAD	O3'-C3'-C4'-C5'
3	A	460	NAD	C5B-O5B-PA-O1A
3	A	460	NAD	O4B-C4B-C5B-O5B
2	A	459	FAD	O4B-C4B-C5B-O5B

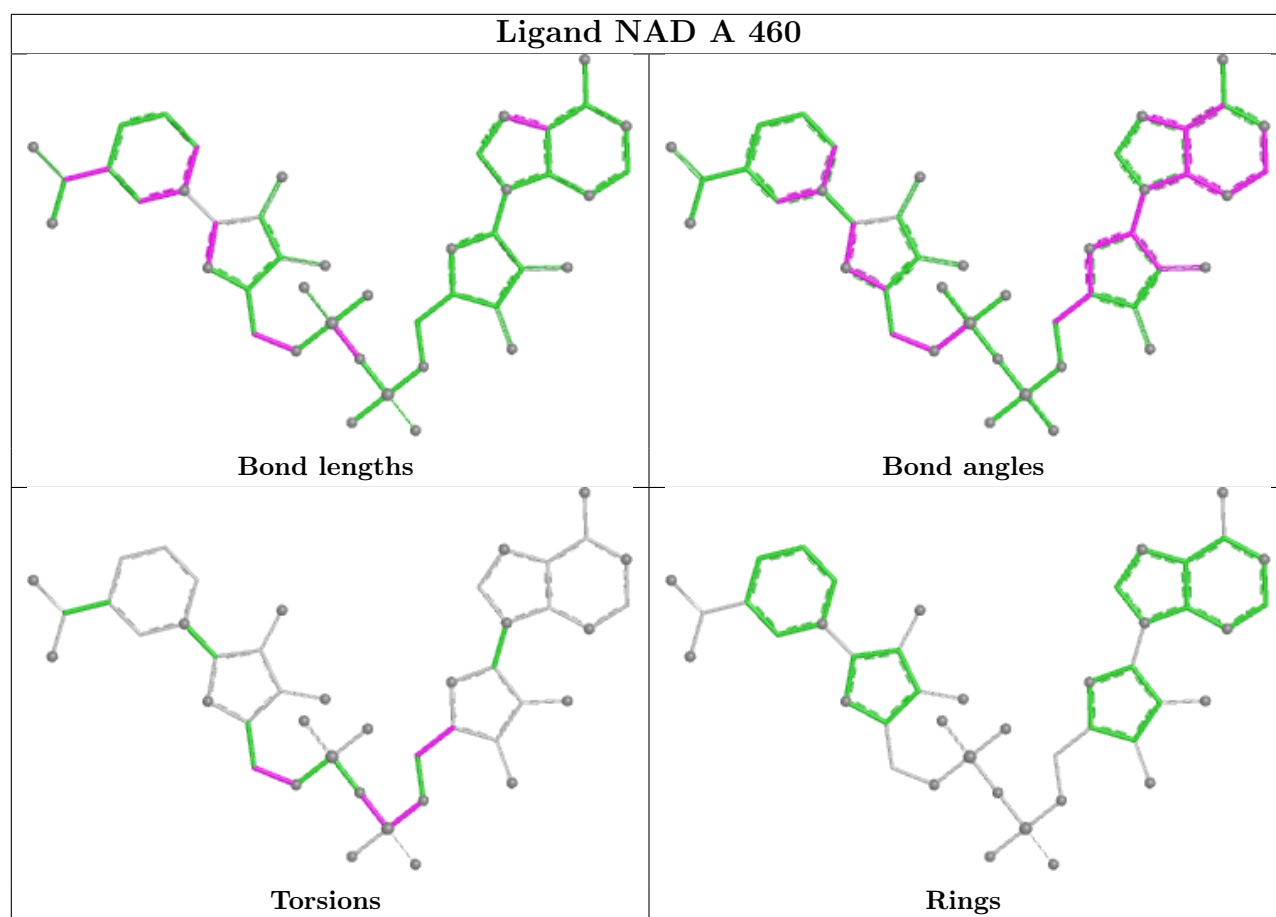
There are no ring outliers.

2 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	459	FAD	2	0
3	A	460	NAD	7	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





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%)	0.50	38 (8%)	17 15	11, 38, 77, 90	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	195	ALA	4.5
1	A	425	ALA	4.5
1	A	398	HIS	3.8
1	A	331	ALA	3.7
1	A	78	ALA	3.7
1	A	242	CYS	3.6
1	A	330	LYS	3.5
1	A	364	LEU	3.2
1	A	25	GLY	3.1
1	A	397	ASN	3.0
1	A	80	PRO	3.0
1	A	326	ILE	2.9
1	A	83	ASP	2.8
1	A	68	THR	2.7
1	A	85	GLY	2.7
1	A	360	SER	2.7
1	A	169	ALA	2.7
1	A	69	GLU	2.6
1	A	248	GLY	2.5
1	A	294	GLN	2.4
1	A	295	THR	2.4
1	A	420	SER	2.4
1	A	173	HIS	2.3
1	A	278	LEU	2.3
1	A	241	GLY	2.2
1	A	240	ASN	2.2
1	A	325	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	396	ASP	2.2
1	A	257	ALA	2.1
1	A	250	GLY	2.1
1	A	71	SER	2.1
1	A	124	LYS	2.1
1	A	431	ALA	2.1
1	A	424	GLY	2.1
1	A	156	GLY	2.1
1	A	171	PRO	2.1
1	A	301	TRP	2.0
1	A	2	GLN	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

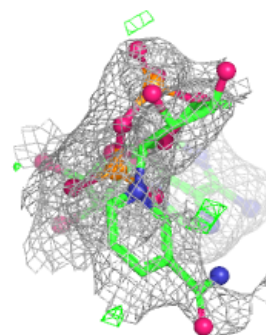
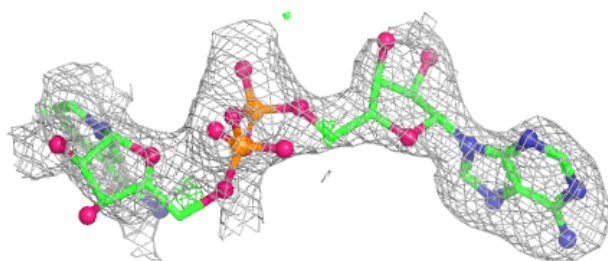
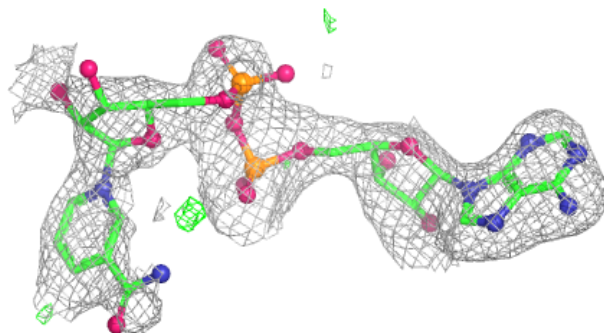
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	NAD	A	460	44/44	0.87	0.11	55,72,90,90	0
2	FAD	A	459	53/53	0.94	0.08	4,27,62,68	0

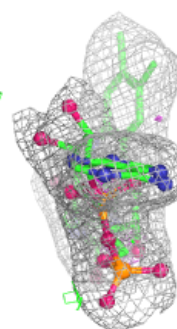
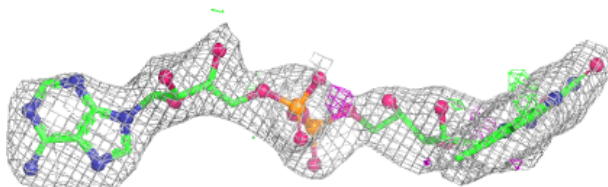
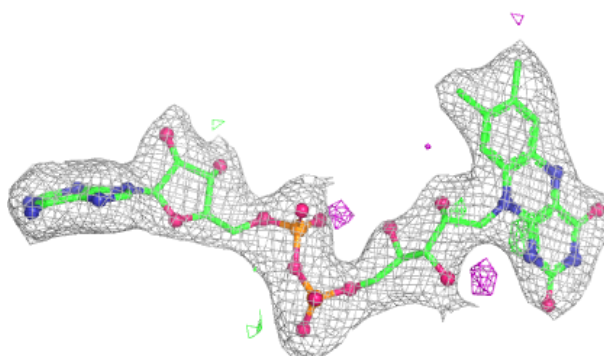
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around NAD A 460:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around FAD A 459:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.