



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 08:40 PM UTC

PDB ID : 3FX2 / pdb_00003fx2
Title : COMPARISON OF THE CRYSTAL STRUCTURES OF A FLAVODOXIN
IN ITS THREE OXIDATION STATES AT CRYOGENIC TEMPERATURES
Authors : Watt, W.; Watenpaugh, K.D.
Deposited on : 1991-10-17
Resolution : 1.90 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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

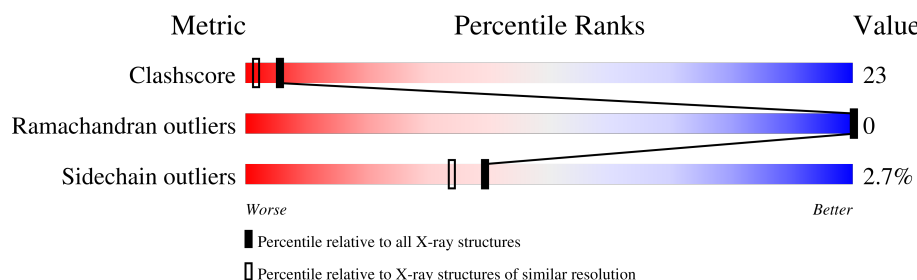
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	147	22% 42% 35% .

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	FMN	A	149	X	X	-	-

2 Entry composition [i](#)

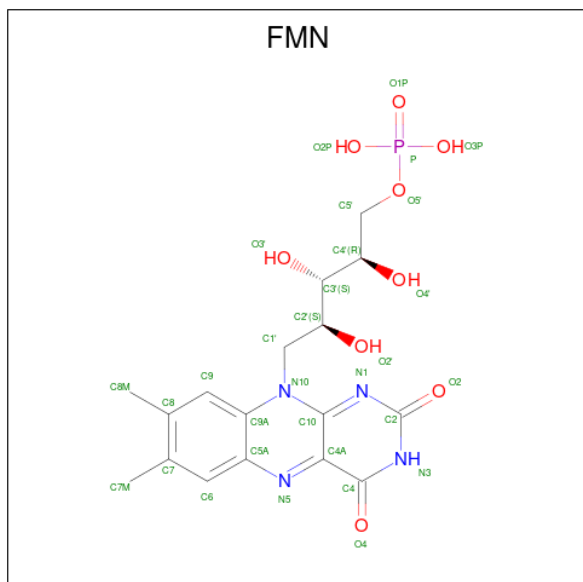
There are 3 unique types of molecules in this entry. The entry contains 1386 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 FLAVODOXIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	147	Total	C	N	O	S	0	0	0
			1102	684	181	233	4			

- Molecule 2 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $C_{17}H_{21}N_4O_9P$).

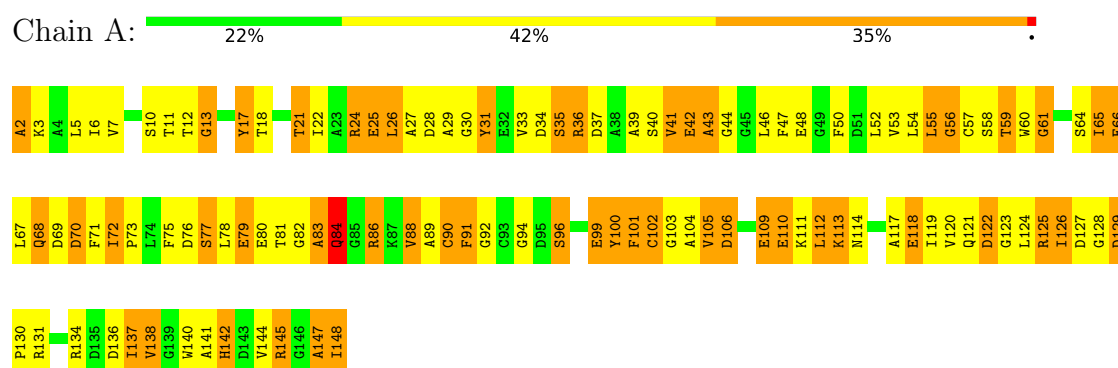


3 Residue-property plots

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. 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. 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.

Note EDS was not executed.

• Molecule 1: FLAVODOXIN



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	50.72Å 50.72Å 139.04Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 1.90	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-1.90)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.199 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	1386	wwPDB-VP
Average B, all atoms (Å ²)	14.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FMN

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	2.47	53/1119 (4.7%)	3.37	164/1514 (10.8%)

All (53) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	145	ARG	CD-NE	-12.54	1.28	1.46
1	A	56	GLY	CA-C	10.84	1.60	1.52
1	A	61	GLY	N-CA	9.67	1.59	1.45
1	A	101	PHE	C-O	9.33	1.35	1.24
1	A	59	THR	CB-OG1	9.31	1.58	1.43
1	A	60	TRP	N-CA	8.90	1.57	1.46
1	A	69	ASP	C-O	8.34	1.33	1.24
1	A	145	ARG	CZ-NH1	8.25	1.44	1.32
1	A	57	CYS	N-CA	7.86	1.54	1.46
1	A	72	ILE	CA-CB	7.83	1.64	1.54
1	A	104	ALA	CA-C	7.55	1.62	1.52
1	A	55	LEU	N-CA	7.47	1.55	1.46
1	A	68	GLN	CD-NE2	-7.34	1.17	1.33
1	A	122	ASP	N-CA	7.26	1.55	1.45
1	A	126	ILE	CB-CG1	7.24	1.68	1.53
1	A	119	ILE	N-CA	7.18	1.54	1.46
1	A	54	LEU	CA-C	7.15	1.61	1.52
1	A	131	ARG	CZ-NH2	7.10	1.42	1.33
1	A	90	CYS	N-CA	7.02	1.54	1.45
1	A	65	ILE	N-CA	6.91	1.54	1.46
1	A	11	THR	CB-OG1	6.88	1.54	1.43
1	A	59	THR	CA-C	6.83	1.61	1.52
1	A	57	CYS	C-O	6.79	1.32	1.23
1	A	120	VAL	CA-CB	6.76	1.62	1.54
1	A	89	ALA	CA-C	6.69	1.60	1.52
1	A	79	GLU	CA-CB	-6.43	1.41	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	122	ASP	CA-CB	-6.40	1.43	1.53
1	A	86	ARG	C-O	6.37	1.31	1.23
1	A	94	GLY	C-O	6.37	1.30	1.23
1	A	102	CYS	CA-CB	6.09	1.63	1.53
1	A	40	SER	CB-OG	6.08	1.54	1.42
1	A	145	ARG	CA-CB	-5.99	1.44	1.53
1	A	13	GLY	C-O	5.98	1.32	1.23
1	A	65	ILE	C-O	-5.84	1.17	1.24
1	A	31	TYR	N-CA	5.79	1.53	1.45
1	A	100	TYR	N-CA	-5.78	1.38	1.46
1	A	79	GLU	N-CA	5.75	1.53	1.46
1	A	104	ALA	C-N	-5.69	1.26	1.33
1	A	120	VAL	CA-C	-5.67	1.45	1.52
1	A	88	VAL	C-N	5.56	1.40	1.33
1	A	26	LEU	C-O	5.55	1.30	1.24
1	A	103	GLY	C-O	5.54	1.30	1.24
1	A	113	LYS	C-O	5.50	1.30	1.24
1	A	105	VAL	N-CA	5.44	1.52	1.46
1	A	125	ARG	N-CA	5.41	1.54	1.46
1	A	11	THR	C-N	-5.38	1.26	1.33
1	A	6	ILE	CB-CG1	5.35	1.64	1.53
1	A	136	ASP	C-N	-5.32	1.27	1.33
1	A	2	ALA	N-CA	5.24	1.56	1.46
1	A	21	THR	CA-CB	5.23	1.61	1.53
1	A	29	ALA	C-N	-5.23	1.26	1.33
1	A	66	GLU	CA-CB	5.10	1.63	1.53
1	A	128	GLY	C-O	-5.03	1.18	1.23

All (164) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	145	ARG	CD-NE-CZ	33.47	171.26	124.40
1	A	79	GLU	CA-CB-CG	17.40	148.90	114.10
1	A	48	GLU	CB-CG-CD	13.84	136.13	112.60
1	A	136	ASP	O-C-N	13.77	136.72	122.12
1	A	145	ARG	CB-CG-CD	-13.59	80.05	111.30
1	A	122	ASP	CA-CB-CG	12.61	125.21	112.60
1	A	142	HIS	CA-CB-CG	-12.19	101.61	113.80
1	A	137	ILE	O-C-N	12.00	134.30	121.94
1	A	56	GLY	O-C-N	11.99	134.75	123.48
1	A	141	ALA	CA-C-O	11.90	133.17	120.55
1	A	47	PHE	CA-CB-CG	11.41	125.21	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	138	VAL	CA-C-N	10.99	132.18	119.98
1	A	138	VAL	C-N-CA	10.99	132.18	119.98
1	A	122	ASP	CB-CA-C	10.85	129.42	109.46
1	A	129	ASP	O-C-N	10.71	130.41	121.31
1	A	145	ARG	CG-CD-NE	10.13	134.29	112.00
1	A	35	SER	CB-CA-C	9.71	125.92	110.19
1	A	28	ASP	CA-CB-CG	9.56	122.16	112.60
1	A	111	LYS	O-C-N	9.38	132.06	122.12
1	A	145	ARG	O-C-N	9.20	131.55	122.07
1	A	84	GLN	CG-CD-NE2	-8.97	102.95	116.40
1	A	12	THR	O-C-N	8.94	133.25	122.26
1	A	25	GLU	CB-CA-C	-8.73	97.17	110.88
1	A	22	ILE	CA-C-O	-8.64	111.97	120.95
1	A	141	ALA	CA-C-N	8.29	131.59	120.65
1	A	141	ALA	C-N-CA	8.29	131.59	120.65
1	A	54	LEU	O-C-N	8.26	133.01	123.27
1	A	36	ARG	NE-CZ-NH2	8.14	126.53	119.20
1	A	86	ARG	NE-CZ-NH1	-8.14	113.36	121.50
1	A	43	ALA	N-CA-C	8.02	120.02	111.28
1	A	91	PHE	CA-C-N	-7.97	110.56	120.92
1	A	91	PHE	C-N-CA	-7.97	110.56	120.92
1	A	89	ALA	N-CA-CB	7.82	125.30	111.69
1	A	137	ILE	CA-C-O	-7.82	112.93	121.29
1	A	7	VAL	CA-C-O	-7.62	112.40	120.48
1	A	59	THR	O-C-N	7.60	132.24	123.27
1	A	136	ASP	CA-C-O	-7.60	112.42	120.63
1	A	118	GLU	CA-CB-CG	7.59	129.28	114.10
1	A	39	ALA	CA-C-N	7.56	134.96	121.66
1	A	39	ALA	C-N-CA	7.56	134.96	121.66
1	A	24	ARG	CA-C-O	-7.54	112.43	120.42
1	A	144	VAL	N-CA-CB	7.54	121.88	110.58
1	A	119	ILE	CA-C-O	-7.53	111.50	120.76
1	A	69	ASP	N-CA-C	7.50	123.74	111.37
1	A	18	THR	O-C-N	7.44	129.73	122.07
1	A	121	GLN	O-C-N	7.38	131.75	123.48
1	A	84	GLN	N-CA-CB	-7.37	98.41	109.69
1	A	25	GLU	CB-CG-CD	-7.35	100.11	112.60
1	A	136	ASP	CA-CB-CG	-7.24	105.36	112.60
1	A	119	ILE	CB-CA-C	7.12	118.92	111.23
1	A	22	ILE	O-C-N	7.12	128.77	121.87
1	A	7	VAL	CA-C-N	-7.04	110.68	122.29
1	A	7	VAL	C-N-CA	-7.04	110.68	122.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	91	PHE	O-C-N	7.04	131.27	123.25
1	A	121	GLN	CA-CB-CG	7.00	128.09	114.10
1	A	88	VAL	CA-C-O	6.97	128.66	121.28
1	A	35	SER	O-C-N	-6.88	115.38	123.22
1	A	94	GLY	CA-C-O	6.86	127.83	121.38
1	A	64	SER	CA-C-N	-6.84	113.82	122.37
1	A	64	SER	C-N-CA	-6.84	113.82	122.37
1	A	66	GLU	CA-CB-CG	-6.80	100.51	114.10
1	A	17	TYR	CA-C-O	6.77	127.60	120.42
1	A	83	ALA	N-CA-C	6.76	120.75	112.23
1	A	77	SER	N-CA-C	6.72	121.08	113.02
1	A	134	ARG	N-CA-CB	6.67	120.07	110.06
1	A	89	ALA	O-C-N	6.66	131.23	123.17
1	A	110	GLU	CA-C-N	-6.50	111.57	120.28
1	A	110	GLU	C-N-CA	-6.50	111.57	120.28
1	A	58	SER	CA-C-O	6.48	129.46	121.81
1	A	137	ILE	N-CA-CB	6.46	117.66	110.62
1	A	113	LYS	CB-CA-C	-6.38	100.60	110.81
1	A	145	ARG	NE-CZ-NH2	6.37	124.93	119.20
1	A	54	LEU	CA-C-O	-6.35	113.33	120.32
1	A	27	ALA	CB-CA-C	6.35	120.85	110.88
1	A	18	THR	OG1-CB-CG2	6.34	121.98	109.30
1	A	30	GLY	CA-C-O	-6.33	111.95	118.97
1	A	119	ILE	O-C-N	6.30	129.55	122.68
1	A	82	GLY	CA-C-N	6.25	131.31	120.68
1	A	82	GLY	C-N-CA	6.25	131.31	120.68
1	A	79	GLU	CG-CD-OE2	-6.24	104.05	118.40
1	A	36	ARG	CA-C-O	-6.21	113.43	120.32
1	A	33	VAL	N-CA-C	6.19	116.79	107.75
1	A	55	LEU	CA-C-N	6.19	126.85	122.33
1	A	55	LEU	C-N-CA	6.19	126.85	122.33
1	A	110	GLU	CA-C-O	6.16	127.08	120.55
1	A	76	ASP	CA-C-O	-6.14	114.00	120.63
1	A	60	TRP	CA-C-N	-6.12	109.40	121.41
1	A	60	TRP	C-N-CA	-6.12	109.40	121.41
1	A	145	ARG	NE-CZ-NH1	-6.12	115.38	121.50
1	A	70	ASP	CA-C-N	6.09	128.94	120.29
1	A	70	ASP	C-N-CA	6.09	128.94	120.29
1	A	58	SER	N-CA-CB	6.05	119.65	110.45
1	A	75	PHE	CA-C-N	-6.05	112.09	120.38
1	A	75	PHE	C-N-CA	-6.05	112.09	120.38
1	A	112	LEU	O-C-N	6.05	128.38	122.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	121	GLN	CA-C-N	-6.02	111.40	121.39
1	A	121	GLN	C-N-CA	-6.02	111.40	121.39
1	A	68	GLN	CA-CB-CG	6.01	126.12	114.10
1	A	128	GLY	O-C-N	5.99	128.05	122.90
1	A	99	GLU	CB-CG-CD	5.97	122.75	112.60
1	A	140	TRP	CA-C-N	5.95	128.26	120.28
1	A	140	TRP	C-N-CA	5.95	128.26	120.28
1	A	86	ARG	NH1-CZ-NH2	5.95	127.03	119.30
1	A	84	GLN	OE1-CD-NE2	5.94	128.54	122.60
1	A	84	GLN	O-C-N	-5.84	115.70	122.95
1	A	2	ALA	O-C-N	5.84	132.35	123.00
1	A	96	SER	N-CA-C	5.82	119.85	112.87
1	A	29	ALA	N-CA-CB	5.80	119.57	110.46
1	A	148	ILE	CA-CB-CG2	5.77	120.32	110.50
1	A	110	GLU	CG-CD-OE1	5.76	131.65	118.40
1	A	99	GLU	CG-CD-OE1	5.73	131.58	118.40
1	A	78	LEU	CA-C-O	5.71	126.60	120.20
1	A	92	GLY	CA-C-O	5.67	126.93	121.49
1	A	30	GLY	N-CA-C	-5.65	106.86	115.00
1	A	109	GLU	N-CA-CB	5.61	118.30	109.94
1	A	59	THR	N-CA-CB	5.53	119.23	110.55
1	A	39	ALA	CA-C-O	5.52	127.10	120.92
1	A	103	GLY	N-CA-C	-5.52	107.48	114.16
1	A	24	ARG	NE-CZ-NH2	-5.51	114.24	119.20
1	A	42	GLU	CA-CB-CG	-5.50	103.09	114.10
1	A	71	PHE	N-CA-C	5.50	117.36	111.36
1	A	142	HIS	CB-CG-ND1	-5.49	114.46	122.70
1	A	22	ILE	N-CA-CB	5.48	117.99	110.54
1	A	121	GLN	CB-CG-CD	5.47	121.91	112.60
1	A	2	ALA	CA-C-N	-5.45	115.42	123.05
1	A	2	ALA	C-N-CA	-5.45	115.42	123.05
1	A	26	LEU	CA-C-N	5.45	127.53	120.44
1	A	26	LEU	C-N-CA	5.45	127.53	120.44
1	A	24	ARG	CD-NE-CZ	5.44	132.02	124.40
1	A	148	ILE	N-CA-CB	5.44	120.75	111.50
1	A	21	THR	CA-C-O	-5.43	115.12	120.82
1	A	21	THR	CA-CB-CG2	5.42	119.71	110.50
1	A	120	VAL	CA-C-O	5.41	126.14	119.43
1	A	90	CYS	O-C-N	5.36	129.84	123.24
1	A	138	VAL	O-C-N	-5.36	116.58	121.94
1	A	55	LEU	N-CA-CB	-5.33	102.20	110.57
1	A	54	LEU	CA-C-N	-5.30	115.69	123.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	54	LEU	C-N-CA	-5.30	115.69	123.00
1	A	65	ILE	O-C-N	-5.28	116.50	122.94
1	A	147	ALA	O-C-N	5.27	128.57	122.19
1	A	106	ASP	OD1-CG-OD2	-5.25	110.30	122.90
1	A	60	TRP	N-CA-CB	-5.25	101.62	110.49
1	A	86	ARG	CA-C-N	5.21	129.27	121.72
1	A	86	ARG	C-N-CA	5.21	129.27	121.72
1	A	67	LEU	N-CA-CB	-5.21	102.68	110.17
1	A	66	GLU	CA-C-O	5.19	126.08	120.32
1	A	114	ASN	CA-CB-CG	-5.18	107.42	112.60
1	A	11	THR	N-CA-CB	5.18	118.21	110.14
1	A	67	LEU	CA-C-O	-5.17	115.92	121.56
1	A	99	GLU	CA-C-N	5.15	130.95	123.12
1	A	99	GLU	C-N-CA	5.15	130.95	123.12
1	A	54	LEU	CB-CG-CD2	-5.13	95.32	110.70
1	A	104	ALA	N-CA-CB	5.11	117.73	110.16
1	A	71	PHE	CA-CB-CG	-5.11	108.69	113.80
1	A	72	ILE	CA-C-N	5.10	124.54	119.24
1	A	72	ILE	C-N-CA	5.10	124.54	119.24
1	A	104	ALA	CA-C-O	-5.10	115.02	120.42
1	A	7	VAL	O-C-N	5.08	128.52	123.18
1	A	76	ASP	CA-C-N	5.08	131.30	122.56
1	A	76	ASP	C-N-CA	5.08	131.30	122.56
1	A	60	TRP	CA-C-O	-5.08	113.25	120.51
1	A	106	ASP	CA-CB-CG	5.05	117.65	112.60
1	A	44	GLY	O-C-N	5.05	129.26	122.70
1	A	89	ALA	CA-C-O	-5.03	115.72	121.40

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	1102	0	1029	50	0
2	A	31	0	18	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	253	0	0	13	0
All	All	1386	0	1047	51	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 23.

All (51) 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:A:68:GLN:HE22	1:A:70:ASP:HB2	1.32	0.93
1:A:25:GLU:OE2	3:A:307:HOH:O	1.89	0.91
1:A:79:GLU:OE2	3:A:271:HOH:O	2.03	0.75
1:A:118:GLU:OE1	3:A:392:HOH:O	2.04	0.74
1:A:99:GLU:HG2	3:A:341:HOH:O	1.88	0.74
1:A:24:ARG:HD3	3:A:368:HOH:O	1.87	0.72
1:A:56:GLY:HA2	1:A:91:PHE:O	1.94	0.68
1:A:110:GLU:OE2	3:A:349:HOH:O	2.11	0.67
1:A:72:ILE:HB	1:A:73:PRO:HD3	1.78	0.66
1:A:110:GLU:OE1	3:A:350:HOH:O	2.15	0.64
1:A:42:GLU:O	1:A:46:LEU:HB2	1.99	0.62
1:A:96:SER:OG	1:A:127:ASP:OD2	2.18	0.62
1:A:10:SER:OG	1:A:13:GLY:HA2	2.01	0.59
1:A:113:LYS:NZ	3:A:401:HOH:O	2.31	0.58
1:A:31:TYR:OH	1:A:148:ILE:HD11	2.04	0.57
1:A:147:ALA:HA	3:A:321:HOH:O	2.06	0.56
1:A:61:GLY:CA	1:A:66:GLU:HG3	2.38	0.54
1:A:5:LEU:HB3	1:A:53:VAL:HG22	1.90	0.53
1:A:90:CYS:O	1:A:123:GLY:HA2	2.07	0.52
1:A:105:VAL:O	1:A:109:GLU:HG3	2.10	0.52
1:A:55:LEU:HD12	1:A:112:LEU:HD11	1.92	0.52
1:A:83:ALA:O	1:A:117:ALA:HB2	2.10	0.51
1:A:126:ILE:HG21	1:A:130:PRO:HB3	1.92	0.51
1:A:10:SER:OG	1:A:13:GLY:CA	2.59	0.51
1:A:31:TYR:CE1	1:A:145:ARG:HG2	2.46	0.50
1:A:43:ALA:O	1:A:81:THR:HA	2.12	0.50
1:A:88:VAL:HG21	1:A:112:LEU:HD13	1.94	0.49
1:A:2:ALA:N	3:A:288:HOH:O	2.44	0.49
1:A:68:GLN:NE2	1:A:70:ASP:HB2	2.15	0.49
1:A:65:ILE:HG13	1:A:100:TYR:CD2	2.48	0.48
1:A:26:LEU:O	1:A:31:TYR:HB2	2.14	0.48
1:A:52:LEU:HD13	1:A:148:ILE:HG21	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:ASP:HB3	3:A:348:HOH:O	2.14	0.47
1:A:77:SER:O	1:A:80:GLU:HG2	2.15	0.47
1:A:124:LEU:HD21	1:A:126:ILE:HD11	1.97	0.46
1:A:34:ASP:CG	1:A:36:ARG:HE	2.25	0.45
1:A:130:PRO:HB2	1:A:137:ILE:HD11	1.97	0.45
1:A:5:LEU:HB2	1:A:50:PHE:CD1	2.51	0.45
1:A:72:ILE:CB	1:A:73:PRO:HD3	2.46	0.44
1:A:129:ASP:OD1	1:A:130:PRO:HD2	2.18	0.44
1:A:84:GLN:C	1:A:86:ARG:H	2.25	0.43
1:A:101:PHE:CZ	1:A:127:ASP:HB2	2.52	0.43
2:A:149:FMN:HM83	2:A:149:FMN:HM71	1.82	0.42
1:A:106:ASP:OD1	1:A:125:ARG:NH2	2.46	0.42
1:A:3:LYS:HE3	3:A:287:HOH:O	2.19	0.42
1:A:59:THR:OG1	1:A:102:CYS:HA	2.19	0.42
1:A:147:ALA:HB2	3:A:321:HOH:O	2.20	0.42
1:A:138:VAL:O	1:A:142:HIS:HB2	2.21	0.40
1:A:21:THR:HB	1:A:137:ILE:HG21	2.04	0.40
1:A:17:TYR:CD1	1:A:17:TYR:C	2.98	0.40
1:A:37:ASP:O	1:A:41:VAL:HG13	2.21	0.40

There are no symmetry-related clashes.

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	145/147 (99%)	138 (95%)	7 (5%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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	111/111 (100%)	108 (97%)	3 (3%)	39	34

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	SER
1	A	41	VAL
1	A	84	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	68	GLN
1	A	84	GLN
1	A	121	GLN

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](#)

1 ligand is 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	FMN	A	149	-	33,33,33	2.67	18 (54%)	48,50,50	3.38	30 (62%)

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	FMN	A	149	-	1/1/4/4	6/18/18/18	0/3/3/3

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	149	FMN	C4'-C3'	5.74	1.63	1.53
2	A	149	FMN	P-O1P	5.32	1.67	1.50
2	A	149	FMN	C9A-N10	4.93	1.49	1.41
2	A	149	FMN	C4A-C10	4.13	1.56	1.44
2	A	149	FMN	C7M-C7	3.38	1.57	1.51
2	A	149	FMN	C5A-N5	-3.28	1.33	1.39
2	A	149	FMN	O4'-C4'	3.16	1.50	1.43
2	A	149	FMN	P-O3P	-3.10	1.43	1.54
2	A	149	FMN	O2-C2	3.04	1.30	1.24
2	A	149	FMN	C6-C5A	2.96	1.44	1.40
2	A	149	FMN	P-O5'	-2.90	1.51	1.60
2	A	149	FMN	C9-C8	2.88	1.43	1.39
2	A	149	FMN	O2'-C2'	-2.70	1.37	1.43
2	A	149	FMN	C2'-C3'	-2.46	1.49	1.53
2	A	149	FMN	C4-N3	2.45	1.43	1.38
2	A	149	FMN	C4A-C4	-2.38	1.35	1.44
2	A	149	FMN	C8M-C8	2.15	1.55	1.51
2	A	149	FMN	C1'-C2'	-2.11	1.49	1.52

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	149	FMN	C1'-N10-C9A	-9.57	102.04	120.63
2	A	149	FMN	C4-C4A-N5	8.90	130.51	118.21
2	A	149	FMN	C5A-C9A-N10	-7.37	111.31	117.97
2	A	149	FMN	O4'-C4'-C3'	-5.73	95.84	109.25
2	A	149	FMN	O2-C2-N1	-5.66	112.41	121.80
2	A	149	FMN	O3P-P-O5'	4.97	119.64	106.67
2	A	149	FMN	C5A-N5-C4A	3.80	124.24	118.09
2	A	149	FMN	O2'-C2'-C1'	3.78	125.75	110.20
2	A	149	FMN	O4-C4-C4A	-3.63	116.96	126.53
2	A	149	FMN	O2'-C2'-C3'	3.61	117.69	109.25
2	A	149	FMN	O2P-P-O1P	-3.45	97.40	110.83
2	A	149	FMN	C4-C4A-C10	-3.42	111.07	116.93
2	A	149	FMN	O5'-C5'-C4'	3.35	118.29	109.36
2	A	149	FMN	O2-C2-N3	3.20	124.72	118.58
2	A	149	FMN	C10-C4A-N5	-3.15	118.38	124.81
2	A	149	FMN	O2P-P-O5'	3.10	114.74	106.67
2	A	149	FMN	C9-C9A-N10	3.01	125.91	121.85
2	A	149	FMN	C4A-C4-N3	2.92	120.70	113.25
2	A	149	FMN	C9A-N10-C10	2.86	125.11	120.75
2	A	149	FMN	C6-C5A-N5	-2.79	113.82	118.44
2	A	149	FMN	C4'-C3'-C2'	-2.76	108.97	113.57
2	A	149	FMN	C7M-C7-C8	-2.70	115.25	120.76
2	A	149	FMN	C9A-C5A-N5	2.66	125.28	122.45
2	A	149	FMN	O4'-C4'-C5'	-2.50	104.48	109.99
2	A	149	FMN	C5A-C6-C7	-2.48	116.24	120.83
2	A	149	FMN	C1'-C2'-C3'	2.30	115.89	109.66
2	A	149	FMN	C9A-C9-C8	-2.25	114.70	119.22
2	A	149	FMN	C2'-C1'-N10	2.15	120.38	110.20
2	A	149	FMN	C9-C8-C7	2.06	122.72	119.69
2	A	149	FMN	C6-C7-C8	2.02	122.65	119.69

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	149	FMN	C2'

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	149	FMN	N10-C1'-C2'-O2'
2	A	149	FMN	O2'-C2'-C3'-O3'
2	A	149	FMN	O2'-C2'-C3'-C4'
2	A	149	FMN	O3'-C3'-C4'-C5'

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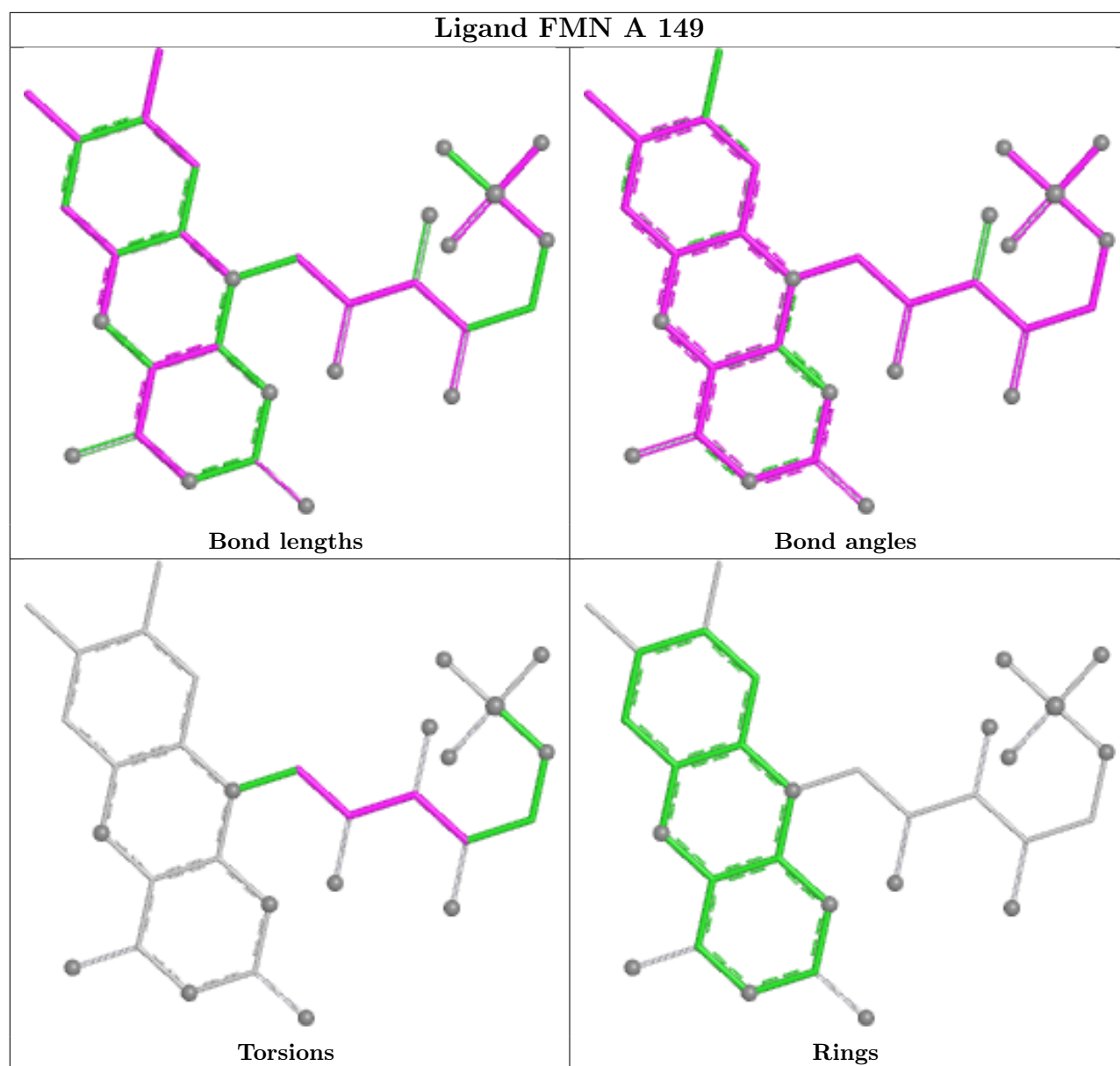
Mol	Chain	Res	Type	Atoms
2	A	149	FMN	C2'-C3'-C4'-C5'
2	A	149	FMN	O3'-C3'-C4'-O4'

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	149	FMN	1	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

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.