



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:45 AM UTC

PDB ID : 5FX2 / pdb_00005fx2
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

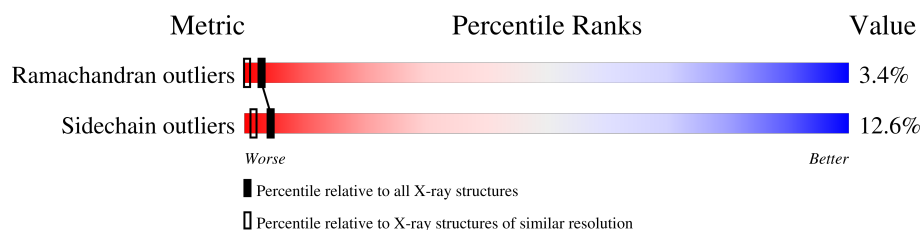
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 Å.

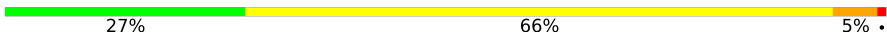
Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
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	

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 1377 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	1102	0	0
			1102	684	181	233	4			

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

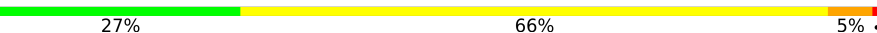


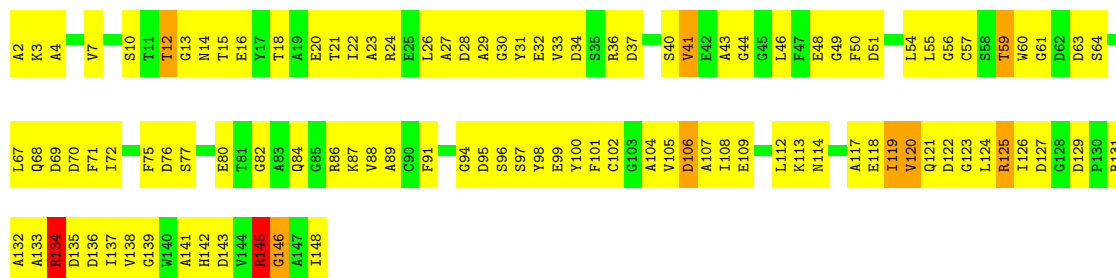
3 Residue-property plots

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

Chain A: 



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	51.36Å 51.36Å 139.38Å 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}	0.213 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	1377	wwPDB-VP
Average B, all atoms (Å ²)	16.0	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	2.02	29/1119 (2.6%)	3.46	199/1514 (13.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	95	ASP	N-CA	8.69	1.56	1.46
1	A	3	LYS	N-CA	-6.84	1.37	1.46
1	A	30	GLY	C-O	6.84	1.31	1.24
1	A	14	ASN	N-CA	-6.75	1.38	1.46
1	A	27	ALA	C-O	6.61	1.32	1.24
1	A	125	ARG	CD-NE	-6.47	1.37	1.46
1	A	118	GLU	C-N	-6.38	1.25	1.33
1	A	69	ASP	C-O	6.31	1.31	1.24
1	A	23	ALA	C-N	-6.22	1.25	1.33
1	A	21	THR	CB-OG1	6.12	1.53	1.43
1	A	57	CYS	N-CA	6.06	1.52	1.46
1	A	143	ASP	CG-OD2	6.02	1.36	1.25
1	A	146	GLY	N-CA	5.97	1.54	1.45
1	A	32	GLU	C-N	-5.94	1.26	1.33
1	A	109	GLU	N-CA	-5.85	1.39	1.46
1	A	68	GLN	C-N	-5.77	1.26	1.33
1	A	91	PHE	C-N	-5.76	1.26	1.32
1	A	71	PHE	N-CA	-5.68	1.38	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	133	ALA	N-CA	5.65	1.52	1.46
1	A	57	CYS	CA-CB	5.59	1.62	1.53
1	A	15	THR	CA-CB	5.43	1.62	1.53
1	A	7	VAL	N-CA	5.38	1.52	1.46
1	A	102	CYS	C-O	5.38	1.30	1.24
1	A	119	ILE	C-N	-5.34	1.28	1.34
1	A	69	ASP	CA-CB	5.29	1.61	1.53
1	A	94	GLY	N-CA	5.24	1.50	1.45
1	A	105	VAL	N-CA	5.10	1.52	1.46
1	A	124	LEU	CA-CB	5.10	1.59	1.53
1	A	60	TRP	CA-CB	5.07	1.61	1.53

All (199) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	136	ASP	CA-CB-CG	19.54	132.14	112.60
1	A	145	ARG	NE-CZ-NH1	15.62	137.12	121.50
1	A	91	PHE	CA-CB-CG	13.05	126.85	113.80
1	A	33	VAL	CA-C-N	12.74	140.56	122.85
1	A	33	VAL	C-N-CA	12.74	140.56	122.85
1	A	108	ILE	CA-C-N	12.48	138.26	120.28
1	A	108	ILE	C-N-CA	12.48	138.26	120.28
1	A	68	GLN	CA-C-N	11.96	138.76	120.82
1	A	68	GLN	C-N-CA	11.96	138.76	120.82
1	A	63	ASP	CA-CB-CG	11.81	124.41	112.60
1	A	75	PHE	CA-C-N	11.36	135.21	120.44
1	A	75	PHE	C-N-CA	11.36	135.21	120.44
1	A	108	ILE	CB-CA-C	11.15	126.15	111.88
1	A	145	ARG	NE-CZ-NH2	-10.24	109.98	119.20
1	A	118	GLU	CA-C-O	-10.17	109.42	120.30
1	A	80	GLU	CA-CB-CG	10.06	134.23	114.10
1	A	122	ASP	CA-CB-CG	-9.85	102.75	112.60
1	A	89	ALA	CB-CA-C	9.64	128.44	109.35
1	A	121	GLN	OE1-CD-NE2	9.51	132.10	122.60
1	A	24	ARG	NE-CZ-NH2	-9.47	110.67	119.20
1	A	26	LEU	CA-C-O	-9.41	111.12	121.00
1	A	24	ARG	NE-CZ-NH1	9.39	130.89	121.50
1	A	24	ARG	CD-NE-CZ	9.35	137.49	124.40
1	A	101	PHE	CA-C-O	-9.31	110.81	120.96
1	A	108	ILE	O-C-N	-9.30	112.64	121.94
1	A	54	LEU	CB-CA-C	9.24	125.86	110.79
1	A	106	ASP	CA-CB-CG	9.19	121.79	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	112	LEU	CB-CA-C	9.13	125.33	110.90
1	A	13	GLY	N-CA-C	9.05	128.19	115.43
1	A	37	ASP	CA-CB-CG	9.04	121.64	112.60
1	A	20	GLU	CB-CG-CD	8.93	127.77	112.60
1	A	141	ALA	CA-C-N	8.93	132.24	120.28
1	A	141	ALA	C-N-CA	8.93	132.24	120.28
1	A	86	ARG	NE-CZ-NH2	8.92	127.23	119.20
1	A	118	GLU	CB-CA-C	-8.92	95.36	110.16
1	A	119	ILE	CB-CG1-CD1	8.90	132.49	113.80
1	A	64	SER	CA-CB-OG	8.87	128.84	111.10
1	A	2	ALA	CA-C-N	8.85	135.44	123.05
1	A	2	ALA	C-N-CA	8.85	135.44	123.05
1	A	145	ARG	CD-NE-CZ	8.79	136.71	124.40
1	A	86	ARG	CA-CB-CG	8.74	131.58	114.10
1	A	75	PHE	CA-C-O	8.74	130.07	120.63
1	A	134	ARG	CA-C-N	8.65	135.38	120.58
1	A	134	ARG	C-N-CA	8.65	135.38	120.58
1	A	61	GLY	CA-C-O	8.62	129.74	122.24
1	A	24	ARG	CA-CB-CG	8.61	131.32	114.10
1	A	13	GLY	CA-C-N	8.58	134.78	120.88
1	A	13	GLY	C-N-CA	8.58	134.78	120.88
1	A	97	SER	CA-CB-OG	8.57	128.23	111.10
1	A	95	ASP	CA-C-O	-8.52	109.74	120.14
1	A	122	ASP	O-C-N	8.52	133.41	122.93
1	A	80	GLU	CG-CD-OE1	8.51	137.98	118.40
1	A	87	LYS	CG-CD-CE	8.44	130.71	111.30
1	A	59	THR	CA-CB-OG1	-8.29	97.16	109.60
1	A	133	ALA	CA-C-N	8.29	137.38	121.54
1	A	133	ALA	C-N-CA	8.29	137.38	121.54
1	A	76	ASP	CA-CB-CG	8.23	120.83	112.60
1	A	43	ALA	N-CA-C	8.22	121.16	111.71
1	A	22	ILE	N-CA-CB	8.21	121.71	110.54
1	A	136	ASP	N-CA-C	-8.17	102.34	111.82
1	A	46	LEU	N-CA-C	8.11	120.84	111.11
1	A	129	ASP	O-C-N	8.04	129.32	121.28
1	A	26	LEU	O-C-N	8.02	130.37	122.03
1	A	7	VAL	O-C-N	8.00	131.58	123.18
1	A	28	ASP	CB-CG-OD2	-7.98	100.04	118.40
1	A	143	ASP	CA-CB-CG	7.98	120.58	112.60
1	A	68	GLN	OE1-CD-NE2	-7.85	114.75	122.60
1	A	15	THR	O-C-N	-7.83	113.06	122.22
1	A	23	ALA	CA-C-N	7.78	130.70	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	23	ALA	C-N-CA	7.78	130.70	120.28
1	A	36	ARG	NE-CZ-NH2	7.73	126.16	119.20
1	A	70	ASP	CA-C-N	7.70	134.62	121.14
1	A	70	ASP	C-N-CA	7.70	134.62	121.14
1	A	56	GLY	N-CA-C	7.66	125.59	111.12
1	A	142	HIS	CA-CB-CG	-7.57	106.23	113.80
1	A	14	ASN	OD1-CG-ND2	-7.56	115.04	122.60
1	A	22	ILE	CA-C-O	-7.55	113.10	120.95
1	A	119	ILE	CA-C-N	7.55	133.17	120.64
1	A	119	ILE	C-N-CA	7.55	133.17	120.64
1	A	129	ASP	N-CA-C	-7.52	98.45	109.50
1	A	137	ILE	N-CA-CB	7.48	120.14	110.57
1	A	80	GLU	CB-CG-CD	7.30	125.02	112.60
1	A	95	ASP	CA-CB-CG	7.28	119.88	112.60
1	A	100	TYR	CA-CB-CG	7.14	126.76	113.90
1	A	137	ILE	CA-C-N	7.08	130.17	120.46
1	A	137	ILE	C-N-CA	7.08	130.17	120.46
1	A	57	CYS	CB-CA-C	-7.08	98.32	109.72
1	A	60	TRP	CA-CB-CG	-7.08	100.15	113.60
1	A	84	GLN	CG-CD-NE2	-7.07	105.80	116.40
1	A	31	TYR	N-CA-CB	-6.98	99.71	109.97
1	A	132	ALA	O-C-N	6.95	130.52	122.25
1	A	120	VAL	CA-C-O	6.88	128.38	119.85
1	A	114	ASN	OD1-CG-ND2	-6.85	115.75	122.60
1	A	121	GLN	CA-C-N	6.84	130.52	120.95
1	A	121	GLN	C-N-CA	6.84	130.52	120.95
1	A	127	ASP	CA-CB-CG	6.71	119.31	112.60
1	A	137	ILE	CB-CA-C	-6.71	103.22	112.02
1	A	88	VAL	CA-CB-CG1	6.70	121.79	110.40
1	A	86	ARG	NE-CZ-NH1	-6.69	114.81	121.50
1	A	51	ASP	CB-CA-C	6.65	123.03	109.67
1	A	133	ALA	N-CA-CB	-6.59	100.33	111.27
1	A	63	ASP	CA-C-N	6.57	132.80	122.94
1	A	63	ASP	C-N-CA	6.57	132.80	122.94
1	A	21	THR	CA-CB-OG1	-6.57	99.75	109.60
1	A	7	VAL	CA-C-O	-6.54	113.55	120.48
1	A	91	PHE	CA-C-N	6.51	130.60	121.22
1	A	91	PHE	C-N-CA	6.51	130.60	121.22
1	A	33	VAL	N-CA-C	6.51	117.40	107.77
1	A	108	ILE	CA-C-O	6.44	127.97	121.27
1	A	69	ASP	N-CA-C	6.44	121.99	111.37
1	A	107	ALA	N-CA-C	-6.41	104.22	111.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	15	THR	CB-CA-C	6.41	122.48	110.63
1	A	50	PHE	CA-CB-CG	-6.39	107.41	113.80
1	A	139	GLY	CA-C-N	6.38	129.35	120.29
1	A	139	GLY	C-N-CA	6.38	129.35	120.29
1	A	100	TYR	CB-CG-CD1	6.35	130.32	120.80
1	A	96	SER	N-CA-CB	6.31	121.02	110.41
1	A	119	ILE	CB-CA-C	6.24	118.38	111.08
1	A	84	GLN	CA-C-O	6.22	127.71	120.49
1	A	67	LEU	CA-C-N	-6.20	111.89	121.56
1	A	67	LEU	C-N-CA	-6.20	111.89	121.56
1	A	67	LEU	O-C-N	6.19	130.22	123.10
1	A	96	SER	O-C-N	6.12	131.36	122.43
1	A	86	ARG	N-CA-CB	6.10	119.72	110.45
1	A	135	ASP	O-C-N	6.09	130.15	122.23
1	A	50	PHE	O-C-N	6.07	131.08	123.19
1	A	36	ARG	N-CA-C	6.06	119.36	109.06
1	A	135	ASP	CB-CA-C	-6.05	99.63	110.70
1	A	121	GLN	CA-CB-CG	6.04	126.18	114.10
1	A	131	ARG	CD-NE-CZ	6.00	132.80	124.40
1	A	95	ASP	O-C-N	5.99	130.25	123.42
1	A	28	ASP	CA-CB-CG	-5.99	106.61	112.60
1	A	100	TYR	CB-CA-C	5.98	120.55	111.70
1	A	61	GLY	O-C-N	-5.91	115.77	122.56
1	A	30	GLY	CA-C-O	5.88	125.15	118.86
1	A	88	VAL	CA-C-O	5.84	126.79	120.43
1	A	113	LYS	CA-C-O	5.83	127.48	121.07
1	A	145	ARG	NH1-CZ-NH2	-5.81	111.75	119.30
1	A	107	ALA	O-C-N	5.78	128.34	122.09
1	A	125	ARG	CD-NE-CZ	5.78	132.49	124.40
1	A	46	LEU	CA-C-N	5.77	130.36	120.72
1	A	46	LEU	C-N-CA	5.77	130.36	120.72
1	A	14	ASN	CB-CG-ND2	5.76	125.05	116.40
1	A	114	ASN	CA-CB-CG	5.73	118.33	112.60
1	A	98	TYR	N-CA-CB	5.72	119.48	110.56
1	A	16	GLU	N-CA-CB	5.65	118.20	110.01
1	A	63	ASP	CA-C-O	5.65	126.51	120.24
1	A	97	SER	N-CA-C	-5.65	105.49	112.38
1	A	126	ILE	N-CA-CB	-5.64	104.57	110.72
1	A	48	GLU	N-CA-C	5.61	122.74	110.80
1	A	55	LEU	CA-C-O	-5.58	113.53	120.57
1	A	21	THR	N-CA-C	-5.57	105.12	111.14
1	A	48	GLU	CB-CG-CD	5.57	122.06	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	109	GLU	CA-C-N	5.57	130.00	120.71
1	A	109	GLU	C-N-CA	5.57	130.00	120.71
1	A	12	THR	N-CA-C	5.54	119.74	112.92
1	A	57	CYS	CA-C-N	5.53	132.93	121.32
1	A	57	CYS	C-N-CA	5.53	132.93	121.32
1	A	18	THR	CA-C-O	-5.50	115.22	121.00
1	A	50	PHE	CA-C-O	-5.49	114.91	121.11
1	A	57	CYS	N-CA-CB	-5.46	101.71	110.77
1	A	99	GLU	N-CA-C	5.46	118.40	111.69
1	A	22	ILE	CA-C-N	5.43	127.50	120.44
1	A	22	ILE	C-N-CA	5.43	127.50	120.44
1	A	16	GLU	CA-C-N	5.43	127.87	120.54
1	A	16	GLU	C-N-CA	5.43	127.87	120.54
1	A	135	ASP	CA-C-O	-5.39	114.25	120.24
1	A	68	GLN	CG-CD-OE1	5.38	131.57	120.80
1	A	4	ALA	CA-C-N	5.38	130.58	123.05
1	A	4	ALA	C-N-CA	5.38	130.58	123.05
1	A	28	ASP	OD1-CG-OD2	5.35	135.75	122.90
1	A	4	ALA	N-CA-CB	-5.35	101.94	111.08
1	A	41	VAL	O-C-N	5.34	129.25	122.57
1	A	18	THR	N-CA-CB	5.33	117.70	109.91
1	A	59	THR	CA-C-O	-5.30	115.17	121.16
1	A	34	ASP	CA-CB-CG	5.29	117.89	112.60
1	A	49	GLY	O-C-N	5.29	129.58	122.70
1	A	67	LEU	CD1-CG-CD2	5.21	122.26	110.80
1	A	104	ALA	O-C-N	5.21	128.09	122.15
1	A	72	ILE	CA-C-N	5.19	124.99	119.28
1	A	72	ILE	C-N-CA	5.19	124.99	119.28
1	A	123	GLY	N-CA-C	-5.17	105.98	111.93
1	A	91	PHE	CA-C-O	-5.17	115.89	121.36
1	A	36	ARG	CG-CD-NE	5.15	123.32	112.00
1	A	145	ARG	N-CA-C	-5.14	103.08	111.04
1	A	96	SER	CA-CB-OG	5.13	121.37	111.10
1	A	143	ASP	CA-C-N	5.10	128.72	121.02
1	A	143	ASP	C-N-CA	5.10	128.72	121.02
1	A	68	GLN	O-C-N	-5.08	117.41	123.11
1	A	57	CYS	N-CA-C	5.08	116.14	108.46
1	A	87	LYS	CB-CA-C	5.06	119.03	110.79
1	A	29	ALA	CA-C-N	5.06	130.34	122.30
1	A	29	ALA	C-N-CA	5.06	130.34	122.30
1	A	15	THR	CA-C-N	5.05	127.01	120.44
1	A	15	THR	C-N-CA	5.05	127.01	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	135	ASP	CA-CB-CG	-5.05	107.55	112.60
1	A	59	THR	O-C-N	5.02	129.49	123.16
1	A	7	VAL	CA-C-N	-5.00	114.81	122.62
1	A	7	VAL	C-N-CA	-5.00	114.81	122.62

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	145	ARG	Sidechain

5.2 Too-close contacts [i](#)

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	0	0
2	A	31	0	19	0	0
3	A	244	0	0	0	0
All	All	1377	0	1048	0	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). Clashscore could not be calculated for this entry.

There are no clashes within the asymmetric unit.

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%)	127 (88%)	13 (9%)	5 (3%)	3 0

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	44	GLY
1	A	117	ALA
1	A	134	ARG
1	A	146	GLY
1	A	82	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	111/111 (100%)	97 (87%)	14 (13%)	4 1

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	SER
1	A	12	THR
1	A	40	SER
1	A	41	VAL
1	A	59	THR
1	A	77	SER
1	A	106	ASP
1	A	119	ILE
1	A	120	VAL
1	A	125	ARG
1	A	134	ARG
1	A	138	VAL
1	A	145	ARG
1	A	148	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	2.34	11 (33%)	48,50,50	3.61	23 (47%)

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	-	2/2/4/4	10/18/18/18	0/3/3/3

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	149	FMN	C1'-C2'	6.12	1.61	1.52
2	A	149	FMN	P-O1P	4.61	1.64	1.50
2	A	149	FMN	C9A-N10	4.60	1.49	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	149	FMN	P-O3P	-4.13	1.39	1.54
2	A	149	FMN	C4A-C10	3.70	1.55	1.44
2	A	149	FMN	C9-C8	3.54	1.44	1.39
2	A	149	FMN	C5A-N5	-2.73	1.34	1.39
2	A	149	FMN	C2'-C3'	2.56	1.57	1.53
2	A	149	FMN	C10-N1	2.47	1.38	1.33
2	A	149	FMN	C5'-C4'	-2.46	1.48	1.51
2	A	149	FMN	O3'-C3'	2.13	1.48	1.43

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	149	FMN	C5A-C9A-N10	-13.10	106.13	117.97
2	A	149	FMN	C1'-N10-C9A	-10.79	99.66	120.63
2	A	149	FMN	C4-C4A-N5	8.09	129.38	118.21
2	A	149	FMN	C9A-C5A-N5	6.28	129.12	122.45
2	A	149	FMN	C5'-C4'-C3'	5.39	122.39	112.22
2	A	149	FMN	C6-C5A-C9A	-5.16	111.96	119.05
2	A	149	FMN	C4'-C3'-C2'	-4.38	106.28	113.57
2	A	149	FMN	C10-C4A-N5	-4.31	116.01	124.81
2	A	149	FMN	C9-C8-C7	-4.31	113.36	119.69
2	A	149	FMN	C4-C4A-C10	-3.63	110.70	116.93
2	A	149	FMN	O4-C4-C4A	-3.10	118.36	126.53
2	A	149	FMN	C9A-N10-C10	2.76	124.96	120.75
2	A	149	FMN	C9-C9A-C5A	2.76	124.91	120.03
2	A	149	FMN	O4'-C4'-C3'	2.68	115.52	109.25
2	A	149	FMN	O2'-C2'-C3'	-2.47	103.46	109.25
2	A	149	FMN	C7M-C7-C8	-2.44	115.77	120.76
2	A	149	FMN	O2-C2-N3	-2.37	114.04	118.58
2	A	149	FMN	C4A-C4-N3	2.36	119.25	113.25
2	A	149	FMN	N3-C2-N1	-2.35	114.51	119.50
2	A	149	FMN	C4A-C10-N10	-2.24	113.27	116.48
2	A	149	FMN	C1'-C2'-C3'	-2.13	103.89	109.66
2	A	149	FMN	O3P-P-O2P	2.11	115.73	107.80
2	A	149	FMN	C8M-C8-C7	-2.08	116.52	120.76

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	149	FMN	C2'
2	A	149	FMN	C3'

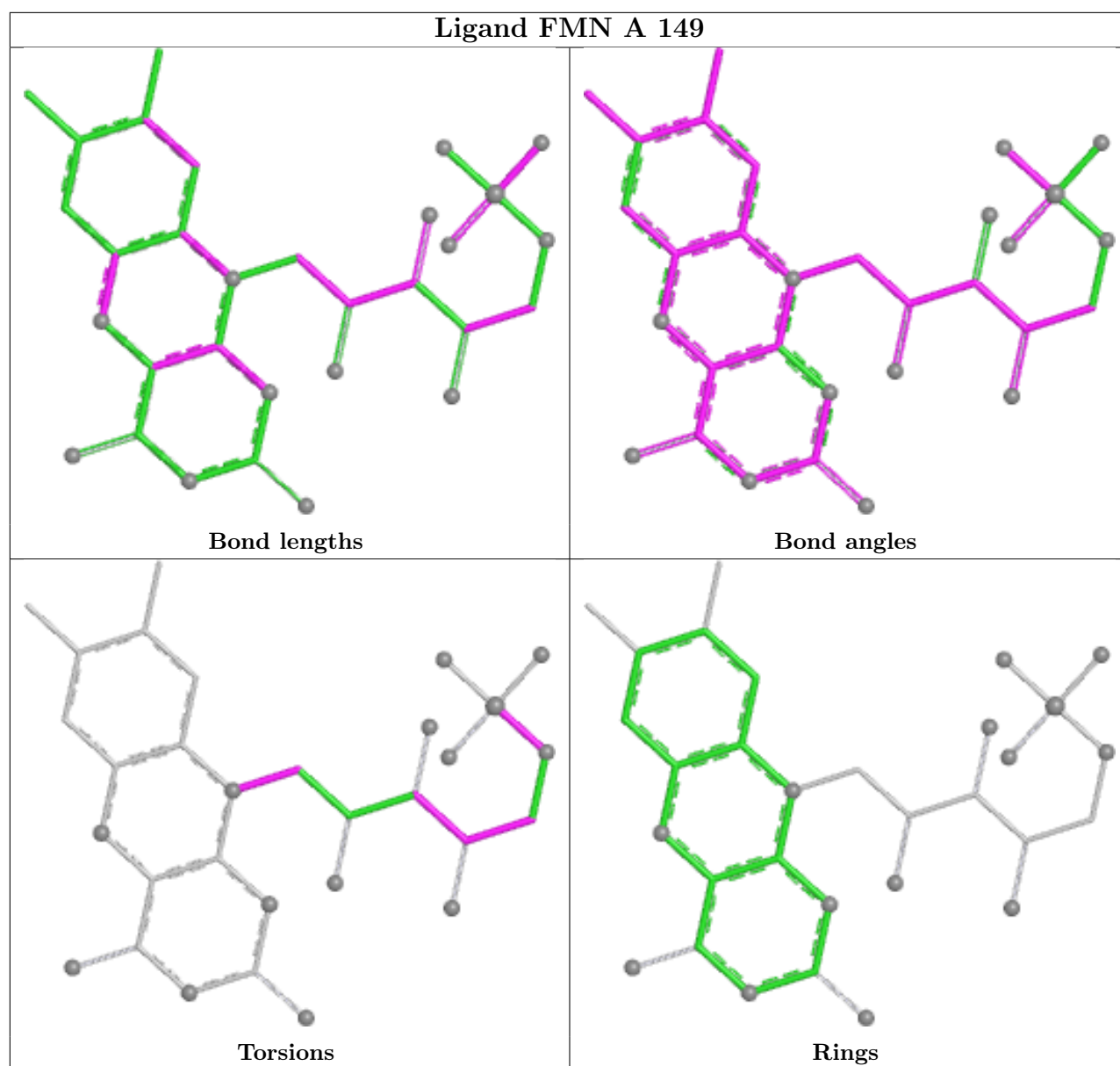
All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	149	FMN	C2'-C1'-N10-C10
2	A	149	FMN	C2'-C3'-C4'-O4'
2	A	149	FMN	C2'-C3'-C4'-C5'
2	A	149	FMN	O3'-C3'-C4'-O4'
2	A	149	FMN	C3'-C4'-C5'-O5'
2	A	149	FMN	O4'-C4'-C5'-O5'
2	A	149	FMN	C5'-O5'-P-O1P
2	A	149	FMN	C5'-O5'-P-O2P
2	A	149	FMN	C5'-O5'-P-O3P
2	A	149	FMN	O3'-C3'-C4'-C5'

There are no ring outliers.

No monomer is involved in short contacts.

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.