



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:23 AM UTC

PDB ID : 1OYC / pdb_00001oyc
Title : OLD YELLOW ENZYME AT 2 ANGSTROMS RESOLUTION: OVERALL
STRUCTURE, LIGAND BINDING AND COMPARISON WITH RELATED
FLAVOPROTEINS
Authors : Fox, K.M.; Karplus, P.A.
Deposited on : 1994-08-25
Resolution : 2.00 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

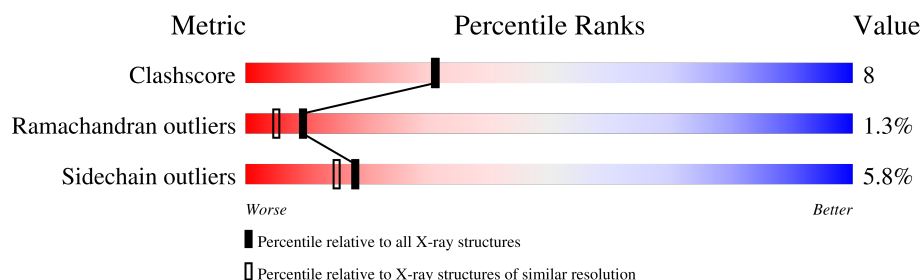
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)

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	400	 52% 36% 10%

2 Entry composition [i](#)

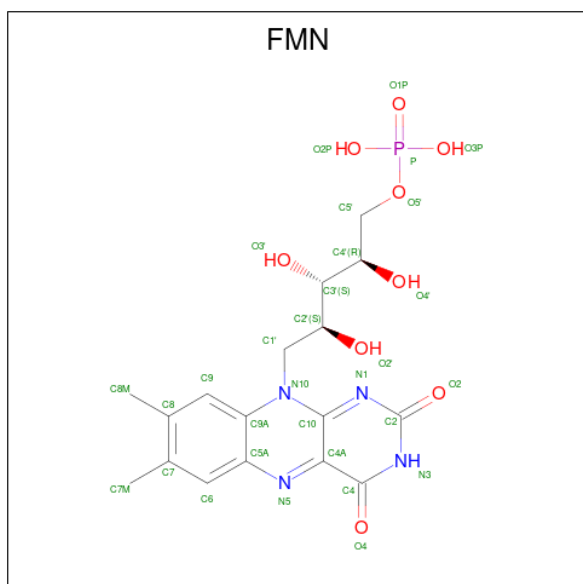
There are 3 unique types of molecules in this entry. The entry contains 4299 atoms, of which 964 are hydrogens and 0 are deuteriums.

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 OLD YELLOW ENZYME.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	399	Total	C	H	N	O	S	4	0	0
			3886	2027	708	551	594	6			

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



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	P	0	0
			35	17	4	4	9	1		

- Molecule 3 is water.

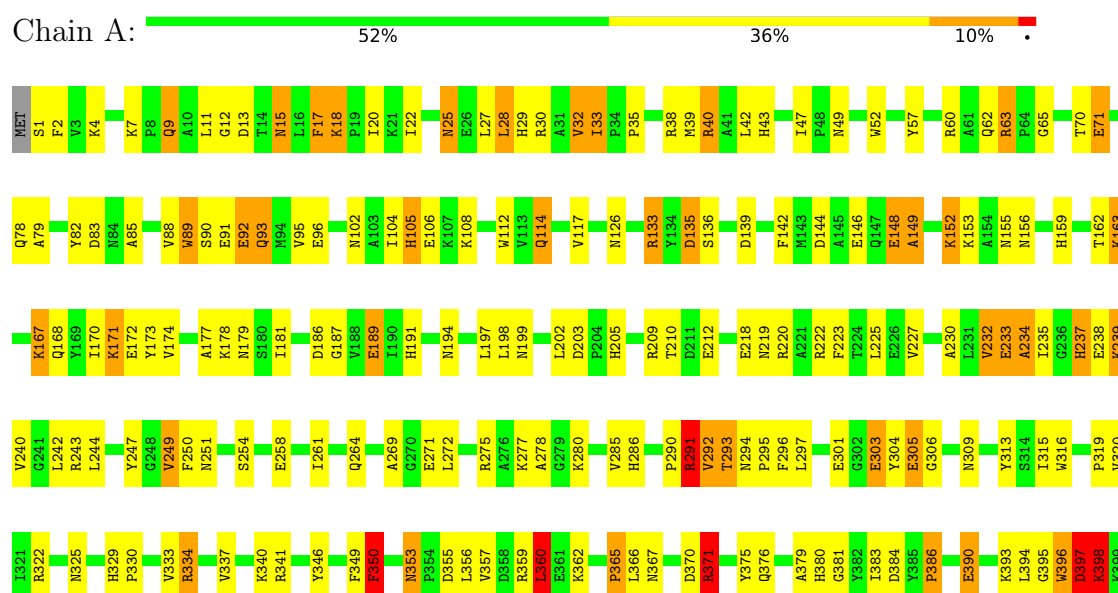
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	126	Total	H	O	0	0
			378	252	126		

3 Residue-property plots [i](#)

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: OLD YELLOW ENZYME



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	142.88Å 142.88Å 43.01Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.00	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.170 , 0.259	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4299	wwPDB-VP
Average B, all atoms (Å ²)	17.0	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	1.60	35/3260 (1.1%)	2.30	190/4417 (4.3%)

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	3

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	105	HIS	CD2-NE2	-9.07	1.27	1.37
1	A	20	ILE	CA-CB	8.92	1.65	1.55
1	A	191	HIS	CD2-NE2	-8.38	1.28	1.37
1	A	375	TYR	C-N	-7.78	1.24	1.33
1	A	159	HIS	CD2-NE2	-7.66	1.29	1.37
1	A	191	HIS	CG-ND1	-7.19	1.30	1.38
1	A	370	ASP	CA-CB	-7.10	1.43	1.53
1	A	95	VAL	CA-CB	-6.94	1.45	1.54
1	A	29	HIS	CG-ND1	-6.75	1.30	1.38
1	A	357	VAL	CA-CB	-6.73	1.46	1.54
1	A	251	ASN	CA-C	-6.42	1.44	1.53
1	A	29	HIS	CD2-NE2	-6.37	1.30	1.37
1	A	280	LYS	CA-CB	-6.04	1.45	1.52
1	A	43	HIS	CD2-NE2	-6.04	1.31	1.37
1	A	247	TYR	CA-C	-6.00	1.44	1.52
1	A	292	VAL	CA-CB	5.92	1.62	1.54
1	A	159	HIS	CG-ND1	-5.92	1.31	1.38
1	A	386	PRO	CA-CB	-5.84	1.47	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	329	HIS	CD2-NE2	-5.75	1.31	1.37
1	A	205	HIS	CD2-NE2	-5.63	1.31	1.37
1	A	237	HIS	CD2-NE2	-5.59	1.31	1.37
1	A	249	VAL	CA-CB	5.49	1.60	1.54
1	A	319	PRO	CA-CB	-5.45	1.46	1.53
1	A	330	PRO	CA-CB	-5.43	1.45	1.53
1	A	38	ARG	CD-NE	-5.43	1.38	1.46
1	A	227	VAL	CA-C	-5.33	1.46	1.52
1	A	261	ILE	CA-CB	5.32	1.61	1.54
1	A	240	VAL	CA-CB	-5.28	1.47	1.54
1	A	162	THR	CA-CB	5.22	1.61	1.53
1	A	205	HIS	CA-CB	-5.13	1.45	1.53
1	A	47	ILE	N-CA	-5.11	1.40	1.46
1	A	9	GLN	CA-CB	-5.09	1.45	1.53
1	A	396	TRP	NE1-CE2	-5.08	1.31	1.37
1	A	316	TRP	NE1-CE2	-5.07	1.31	1.37
1	A	380	HIS	CD2-NE2	-5.07	1.32	1.37

All (190) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	144	ASP	CA-CB-CG	13.04	125.64	112.60
1	A	296	PHE	CA-CB-CG	-12.71	101.09	113.80
1	A	38	ARG	CG-CD-NE	-11.70	86.27	112.00
1	A	371	ARG	CA-CB-CG	10.27	134.65	114.10
1	A	353	ASN	OD1-CG-ND2	-9.91	112.69	122.60
1	A	233	GLU	CB-CG-CD	9.32	128.44	112.60
1	A	249	VAL	N-CA-C	-9.17	104.20	113.10
1	A	146	GLU	CA-CB-CG	8.83	131.75	114.10
1	A	264	GLN	OE1-CD-NE2	-8.81	113.79	122.60
1	A	18	LYS	CA-CB-CG	-8.66	96.78	114.10
1	A	102	ASN	CB-CG-ND2	8.62	129.34	116.40
1	A	38	ARG	NE-CZ-NH2	-8.31	111.72	119.20
1	A	88	VAL	N-CA-CB	-8.31	97.52	111.23
1	A	239	LYS	CA-CB-CG	-8.20	97.69	114.10
1	A	349	PHE	CA-CB-CG	-8.13	105.67	113.80
1	A	330	PRO	N-CA-C	-8.09	103.75	113.86
1	A	93	GLN	OE1-CD-NE2	-8.08	114.52	122.60
1	A	179	ASN	OD1-CG-ND2	-7.95	114.65	122.60
1	A	106	GLU	CA-CB-CG	7.85	129.81	114.10
1	A	179	ASN	CA-CB-CG	7.79	120.39	112.60
1	A	249	VAL	O-C-N	-7.79	114.35	122.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	223	PHE	N-CA-C	-7.76	102.42	111.03
1	A	178	LYS	CA-CB-CG	-7.72	98.67	114.10
1	A	220	ARG	NE-CZ-NH1	7.58	129.08	121.50
1	A	264	GLN	CG-CD-NE2	7.52	127.67	116.40
1	A	135	ASP	N-CA-C	7.48	121.58	110.52
1	A	62	GLN	N-CA-C	7.40	120.79	111.69
1	A	254	SER	N-CA-C	7.38	119.40	111.36
1	A	105	HIS	CB-CG-CD2	-7.25	121.78	131.20
1	A	232	VAL	CA-C-O	-7.24	113.17	120.85
1	A	220	ARG	NE-CZ-NH2	-7.24	112.68	119.20
1	A	329	HIS	CA-CB-CG	-7.24	106.56	113.80
1	A	303	GLU	N-CA-C	-7.18	98.85	110.20
1	A	277	LYS	N-CA-C	-7.12	103.45	111.14
1	A	194	ASN	OD1-CG-ND2	-7.11	115.49	122.60
1	A	398	LYS	N-CA-C	-7.08	95.71	110.80
1	A	52	TRP	CG-CD2-CE3	7.07	140.97	133.90
1	A	227	VAL	CA-C-O	-7.07	113.68	121.17
1	A	133	ARG	NE-CZ-NH2	-7.04	112.86	119.20
1	A	381	GLY	N-CA-C	-7.01	104.29	115.08
1	A	242	LEU	CA-C-O	-6.94	112.62	120.32
1	A	379	ALA	CA-C-O	6.86	127.69	120.42
1	A	291	ARG	NE-CZ-NH1	6.73	128.23	121.50
1	A	57	TYR	N-CA-C	-6.64	103.22	112.45
1	A	210	THR	CB-CA-C	-6.51	99.17	110.17
1	A	91	GLU	CA-CB-CG	6.50	127.10	114.10
1	A	60	ARG	CA-CB-CG	-6.46	101.18	114.10
1	A	159	HIS	CB-CG-CD2	-6.46	122.81	131.20
1	A	78	GLN	OE1-CD-NE2	-6.45	116.15	122.60
1	A	148	GLU	N-CA-CB	-6.45	100.61	110.16
1	A	155	ASN	CB-CG-ND2	-6.38	106.83	116.40
1	A	88	VAL	CB-CA-C	6.36	121.71	111.29
1	A	334	ARG	NE-CZ-NH2	-6.30	113.53	119.20
1	A	322	ARG	CA-C-O	-6.29	114.04	120.71
1	A	396	TRP	CA-C-N	6.25	133.48	121.54
1	A	396	TRP	C-N-CA	6.25	133.48	121.54
1	A	205	HIS	CB-CG-CD2	-6.21	123.13	131.20
1	A	294	ASN	CB-CG-ND2	-6.19	107.12	116.40
1	A	371	ARG	N-CA-C	-6.19	105.22	112.89
1	A	280	LYS	N-CA-C	6.17	119.26	110.68
1	A	360	LEU	N-CA-C	-6.17	104.47	111.14
1	A	162	THR	N-CA-C	-6.14	101.37	110.46
1	A	104	ILE	N-CA-C	-6.12	104.53	110.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	203	ASP	N-CA-C	6.11	117.51	109.93
1	A	220	ARG	CB-CG-CD	-6.10	97.27	111.30
1	A	223	PHE	CA-C-O	-6.08	114.64	120.90
1	A	40	ARG	N-CA-C	-6.07	105.05	112.88
1	A	108	LYS	CB-CG-CD	-6.07	97.35	111.30
1	A	315	ILE	N-CA-C	-6.06	105.78	111.48
1	A	155	ASN	CA-CB-CG	-6.06	106.54	112.60
1	A	52	TRP	CB-CG-CD1	-6.02	117.87	126.90
1	A	269	ALA	CA-C-N	6.01	126.65	119.98
1	A	269	ALA	C-N-CA	6.01	126.65	119.98
1	A	20	ILE	N-CA-C	-6.00	99.22	107.75
1	A	173	TYR	N-CA-C	-6.00	104.66	111.14
1	A	291	ARG	NH1-CZ-NH2	-5.98	111.53	119.30
1	A	220	ARG	CG-CD-NE	-5.95	98.92	112.00
1	A	232	VAL	N-CA-C	-5.93	104.73	110.72
1	A	305	GLU	CB-CG-CD	5.92	122.67	112.60
1	A	371	ARG	CA-C-O	-5.91	111.98	119.31
1	A	355	ASP	N-CA-CB	-5.88	102.67	111.25
1	A	33	ILE	CA-C-N	5.86	126.41	120.38
1	A	33	ILE	C-N-CA	5.86	126.41	120.38
1	A	71	GLU	CA-C-O	-5.85	112.14	120.51
1	A	167	LYS	CG-CD-CE	5.85	124.75	111.30
1	A	225	LEU	O-C-N	-5.84	114.50	122.33
1	A	96	GLU	O-C-N	-5.84	114.51	122.33
1	A	234	ALA	O-C-N	-5.83	116.06	122.07
1	A	199	ASN	CA-CB-CG	5.82	118.42	112.60
1	A	30	ARG	NE-CZ-NH1	5.82	127.32	121.50
1	A	334	ARG	NE-CZ-NH1	5.79	127.29	121.50
1	A	218	GLU	CA-CB-CG	5.77	125.65	114.10
1	A	341	ARG	CA-C-N	5.75	130.41	122.77
1	A	341	ARG	C-N-CA	5.75	130.41	122.77
1	A	42	LEU	CD1-CG-CD2	5.72	123.39	110.80
1	A	383	ILE	CA-C-N	-5.71	113.58	122.67
1	A	383	ILE	C-N-CA	-5.71	113.58	122.67
1	A	126	ASN	OD1-CG-ND2	-5.70	116.90	122.60
1	A	396	TRP	CG-CD2-CE3	5.70	139.60	133.90
1	A	89	TRP	CG-CD2-CE3	5.69	139.59	133.90
1	A	156	ASN	OD1-CG-ND2	-5.66	116.94	122.60
1	A	397	ASP	CA-CB-CG	-5.66	106.94	112.60
1	A	102	ASN	CB-CA-C	-5.66	101.23	110.85
1	A	199	ASN	N-CA-C	-5.63	105.29	111.82
1	A	83	ASP	N-CA-C	5.62	118.34	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	85	ALA	CA-C-N	5.62	125.59	120.03
1	A	85	ALA	C-N-CA	5.62	125.59	120.03
1	A	258	GLU	N-CA-C	-5.62	100.03	108.96
1	A	47	ILE	CA-CB-CG2	-5.58	101.02	110.50
1	A	52	TRP	CE2-CD2-CG	-5.58	100.50	107.20
1	A	70	THR	OG1-CB-CG2	-5.58	98.14	109.30
1	A	384	ASP	CA-CB-CG	5.58	118.17	112.60
1	A	285	VAL	N-CA-C	-5.57	100.45	108.53
1	A	106	GLU	CB-CA-C	-5.57	101.89	110.81
1	A	4	LYS	N-CA-C	5.57	117.82	111.02
1	A	139	ASP	CA-C-N	-5.57	113.80	122.37
1	A	139	ASP	C-N-CA	-5.57	113.80	122.37
1	A	199	ASN	O-C-N	-5.56	115.43	122.27
1	A	375	TYR	O-C-N	-5.55	114.55	122.99
1	A	88	VAL	CG1-CB-CG2	5.55	123.01	110.80
1	A	198	LEU	CD1-CG-CD2	-5.54	98.60	110.80
1	A	32	VAL	CA-C-N	5.54	126.37	122.60
1	A	32	VAL	C-N-CA	5.54	126.37	122.60
1	A	148	GLU	CB-CG-CD	-5.54	103.19	112.60
1	A	91	GLU	CB-CA-C	-5.53	101.46	110.85
1	A	362	LYS	CB-CG-CD	-5.50	98.66	111.30
1	A	237	HIS	CB-CG-CD2	-5.49	124.06	131.20
1	A	170	ILE	CA-C-O	-5.48	115.04	120.85
1	A	329	HIS	CB-CG-CD2	-5.46	124.10	131.20
1	A	187	GLY	CA-C-O	-5.43	116.21	121.75
1	A	114	GLN	OE1-CD-NE2	-5.43	117.17	122.60
1	A	376	GLN	OE1-CD-NE2	-5.42	117.18	122.60
1	A	290	PRO	N-CA-C	-5.42	107.09	113.86
1	A	43	HIS	CB-CG-CD2	-5.40	124.18	131.20
1	A	202	LEU	O-C-N	-5.39	115.64	122.27
1	A	71	GLU	CB-CA-C	-5.38	99.71	110.42
1	A	27	LEU	N-CA-C	-5.38	101.70	110.20
1	A	316	TRP	CG-CD2-CE3	5.37	139.27	133.90
1	A	4	LYS	CB-CA-C	-5.37	102.38	110.92
1	A	177	ALA	CA-C-O	-5.36	114.73	120.42
1	A	380	HIS	CB-CG-CD2	-5.36	124.23	131.20
1	A	17	PHE	CA-CB-CG	-5.35	108.45	113.80
1	A	136	SER	CA-CB-OG	-5.35	100.41	111.10
1	A	250	PHE	CA-CB-CG	5.34	119.14	113.80
1	A	15	ASN	OD1-CG-ND2	-5.34	117.26	122.60
1	A	181	ILE	N-CA-C	-5.34	105.51	110.53
1	A	293	THR	CA-C-O	5.34	125.01	119.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	249	VAL	CG1-CB-CG2	-5.33	99.09	110.80
1	A	92	GLU	CA-CB-CG	5.29	124.69	114.10
1	A	78	GLN	N-CA-C	-5.29	106.08	112.54
1	A	2	PHE	CA-CB-CG	5.29	119.09	113.80
1	A	350	PHE	CA-C-N	5.29	127.31	120.70
1	A	350	PHE	C-N-CA	5.29	127.31	120.70
1	A	309	ASN	O-C-N	-5.26	115.11	122.37
1	A	210	THR	N-CA-CB	5.26	118.55	110.61
1	A	233	GLU	N-CA-CB	5.25	117.93	110.16
1	A	306	GLY	CA-C-O	5.25	123.82	119.04
1	A	39	MET	N-CA-C	5.25	118.82	111.74
1	A	179	ASN	CB-CG-ND2	5.23	124.24	116.40
1	A	393	LYS	O-C-N	-5.23	116.58	122.12
1	A	197	LEU	N-CA-C	5.21	117.38	111.02
1	A	102	ASN	CA-CB-CG	5.21	117.81	112.60
1	A	376	GLN	O-C-N	-5.20	117.86	123.42
1	A	189	GLU	N-CA-C	-5.19	100.44	108.90
1	A	319	PRO	CA-C-O	-5.19	115.08	121.31
1	A	25	ASN	OD1-CG-ND2	-5.19	117.41	122.60
1	A	390	GLU	CB-CG-CD	5.18	121.41	112.60
1	A	320	VAL	O-C-N	-5.16	117.73	123.20
1	A	9	GLN	CB-CG-CD	-5.16	103.83	112.60
1	A	168	GLN	N-CA-C	-5.16	105.74	111.36
1	A	232	VAL	CG1-CB-CG2	-5.16	99.45	110.80
1	A	325	ASN	OD1-CG-ND2	-5.16	117.44	122.60
1	A	380	HIS	CE1-NE2-CD2	5.15	114.15	109.00
1	A	29	HIS	O-C-N	-5.14	118.15	123.29
1	A	172	GLU	N-CA-CB	-5.14	102.31	110.22
1	A	149	ALA	N-CA-C	-5.12	105.59	111.07
1	A	13	ASP	CA-CB-CG	5.11	117.71	112.60
1	A	133	ARG	NE-CZ-NH1	5.11	126.61	121.50
1	A	209	ARG	NE-CZ-NH2	5.07	123.77	119.20
1	A	171	LYS	CG-CD-CE	5.06	122.93	111.30
1	A	15	ASN	CB-CG-ND2	5.05	123.97	116.40
1	A	142	PHE	CA-CB-CG	5.04	118.84	113.80
1	A	102	ASN	OD1-CG-ND2	-5.02	117.58	122.60
1	A	85	ALA	N-CA-C	-5.02	103.22	110.40
1	A	82	TYR	N-CA-C	-5.02	100.72	108.90
1	A	35	PRO	O-C-N	-5.01	117.52	122.98
1	A	397	ASP	O-C-N	5.01	129.26	122.59
1	A	304	TYR	CA-C-N	-5.01	115.71	123.17
1	A	304	TYR	C-N-CA	-5.01	115.71	123.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	168	GLN	CA-C-O	-5.01	115.11	120.42

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	313	TYR	Sidechain
1	A	396	TRP	Mainchain
1	A	397	ASP	Mainchain

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	3178	708	3093	52	0
2	A	31	4	19	1	0
3	A	126	252	0	4	0
All	All	3335	964	3112	52	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 8.

All (52) 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:353:ASN:HD21	1:A:367:ASN:H	1.28	0.80
1:A:9:GLN:NE2	1:A:334:ARG:HH11	1.85	0.74
1:A:114:GLN:HE22	2:A:401:FMN:HN3	1.32	0.74
1:A:28:LEU:HB2	1:A:65:GLY:HA3	1.74	0.70
1:A:295:PRO:HG3	3:A:616:HOH:O	1.93	0.67
1:A:291:ARG:HH11	1:A:291:ARG:HB2	1.62	0.65
1:A:9:GLN:HE21	1:A:334:ARG:NH1	1.98	0.61
1:A:9:GLN:HE21	1:A:334:ARG:HH11	1.47	0.61
1:A:63:ARG:HD2	3:A:583:HOH:O	2.04	0.57
1:A:89:TRP:H	1:A:93:GLN:NE2	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:25:ASN:ND2	1:A:112:TRP:HE1	2.01	0.57
1:A:89:TRP:H	1:A:93:GLN:HE22	1.51	0.57
1:A:133:ARG:HD2	1:A:135:ASP:OD1	2.07	0.55
1:A:105:HIS:HE1	1:A:186:ASP:OD2	1.89	0.55
1:A:333:VAL:O	1:A:337:VAL:HG22	2.09	0.53
1:A:149:ALA:HB1	1:A:153:LYS:HE3	1.91	0.53
1:A:353:ASN:HD22	1:A:359:ARG:CZ	2.22	0.52
1:A:212:GLU:O	1:A:222:ARG:NH1	2.44	0.51
1:A:92:GLU:HG3	3:A:635:HOH:O	2.10	0.51
1:A:356:LEU:HG	1:A:360:LEU:HD22	1.91	0.51
1:A:219:ASN:HA	1:A:222:ARG:NH1	2.28	0.49
1:A:40:ARG:O	1:A:49:ASN:HB2	2.13	0.48
1:A:303:GLU:HB3	1:A:305:GLU:OE2	2.13	0.48
1:A:235:ILE:O	1:A:239:LYS:HE2	2.15	0.47
1:A:163:LYS:HE3	1:A:163:LYS:HB2	1.81	0.47
1:A:249:VAL:HG22	1:A:293:THR:HB	1.97	0.47
1:A:189:GLU:OE2	1:A:286:HIS:HD2	1.98	0.47
1:A:398:LYS:HZ2	1:A:398:LYS:HB3	1.80	0.47
1:A:33:ILE:HG12	1:A:350:PHE:CE2	2.51	0.46
1:A:232:VAL:HG22	1:A:237:HIS:HA	1.98	0.45
1:A:174:VAL:HG13	1:A:234:ALA:HB2	1.99	0.45
1:A:395:GLY:C	1:A:397:ASP:H	2.24	0.45
1:A:397:ASP:O	1:A:398:LYS:HB2	2.15	0.45
1:A:230:ALA:O	1:A:233:GLU:HG3	2.17	0.45
1:A:292:VAL:HG13	3:A:508:HOH:O	2.16	0.44
1:A:359:ARG:HD3	1:A:365:PRO:O	2.18	0.44
1:A:90:SER:H	1:A:93:GLN:NE2	2.16	0.43
1:A:271:GLU:HB3	1:A:275:ARG:NH1	2.33	0.43
1:A:12:GLY:HA2	1:A:17:PHE:CD2	2.52	0.43
1:A:243:ARG:HH21	1:A:286:HIS:CE1	2.35	0.43
1:A:386:PRO:HB2	1:A:390:GLU:HB2	2.00	0.43
1:A:167:LYS:O	1:A:171:LYS:HD3	2.20	0.42
1:A:25:ASN:HD21	1:A:112:TRP:HE1	1.68	0.42
1:A:15:ASN:OD1	1:A:18:LYS:HD2	2.20	0.42
1:A:371:ARG:CZ	1:A:371:ARG:H	2.32	0.42
1:A:22:ILE:HD13	1:A:22:ILE:HA	1.82	0.41
1:A:79:ALA:HB1	1:A:117:VAL:HG22	2.01	0.41
1:A:297:LEU:HB3	1:A:301:GLU:HB2	2.03	0.41
1:A:9:GLN:NE2	1:A:334:ARG:NH1	2.57	0.41
1:A:148:GLU:O	1:A:152:LYS:HG2	2.21	0.40
1:A:346:TYR:CE2	1:A:360:LEU:HD21	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:353:ASN:ND2	1:A:359:ARG:CZ	2.84	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	397/400 (99%)	375 (94%)	17 (4%)	5 (1%)	9 5

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	398	LYS
1	A	71	GLU
1	A	278	ALA
1	A	397	ASP
1	A	365	PRO

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	328/329 (100%)	309 (94%)	19 (6%)	18 15

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	SER
1	A	7	LYS
1	A	11	LEU
1	A	28	LEU
1	A	32	VAL
1	A	63	ARG
1	A	152	LYS
1	A	163	LYS
1	A	238	GLU
1	A	244	LEU
1	A	272	LEU
1	A	291	ARG
1	A	340	LYS
1	A	350	PHE
1	A	360	LEU
1	A	366	LEU
1	A	371	ARG
1	A	394	LEU
1	A	398	LYS

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

Mol	Chain	Res	Type
1	A	9	GLN
1	A	25	ASN
1	A	46	ASN
1	A	84	ASN
1	A	93	GLN
1	A	105	HIS
1	A	114	GLN
1	A	126	ASN
1	A	156	ASN
1	A	175	GLN
1	A	179	ASN
1	A	191	HIS
1	A	200	GLN
1	A	286	HIS
1	A	353	ASN
1	A	380	HIS

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	401	-	33,33,33	1.62	9 (27%)	48,50,50	2.44	17 (35%)

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	401	-	-	4/18/18/18	0/3/3/3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	FMN	C4A-N5	3.61	1.38	1.30
2	A	401	FMN	P-O2P	-2.89	1.44	1.54
2	A	401	FMN	C4'-C3'	-2.89	1.48	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	FMN	P-O1P	-2.51	1.42	1.50
2	A	401	FMN	P-O5'	-2.34	1.52	1.60
2	A	401	FMN	C1'-N10	2.27	1.53	1.47
2	A	401	FMN	C5A-N5	-2.16	1.35	1.39
2	A	401	FMN	C4-N3	2.14	1.42	1.38
2	A	401	FMN	C9A-N10	-2.06	1.37	1.41

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	FMN	C5'-C4'-C3'	-10.16	93.06	112.22
2	A	401	FMN	C4-N3-C2	-4.15	118.28	125.64
2	A	401	FMN	C4-C4A-N5	4.04	123.79	118.21
2	A	401	FMN	O5'-C5'-C4'	-3.53	99.93	109.36
2	A	401	FMN	O3'-C3'-C4'	-3.48	101.03	108.93
2	A	401	FMN	C5A-C9A-N10	3.40	121.05	117.97
2	A	401	FMN	C10-N1-C2	3.22	123.83	116.85
2	A	401	FMN	O3'-C3'-C2'	3.07	115.92	108.93
2	A	401	FMN	C10-C4A-N5	-3.00	118.69	124.81
2	A	401	FMN	O4-C4-N3	-2.80	114.84	120.11
2	A	401	FMN	C8M-C8-C9	-2.71	114.80	119.57
2	A	401	FMN	O2P-P-O1P	2.67	121.24	110.83
2	A	401	FMN	O2'-C2'-C3'	-2.63	103.08	109.25
2	A	401	FMN	C4A-C10-N10	2.47	120.02	116.48
2	A	401	FMN	C4'-C3'-C2'	2.33	117.45	113.57
2	A	401	FMN	C1'-C2'-C3'	2.32	115.94	109.66
2	A	401	FMN	C4A-C10-N1	-2.14	119.33	124.59

There are no chirality outliers.

All (4) torsion outliers are listed below:

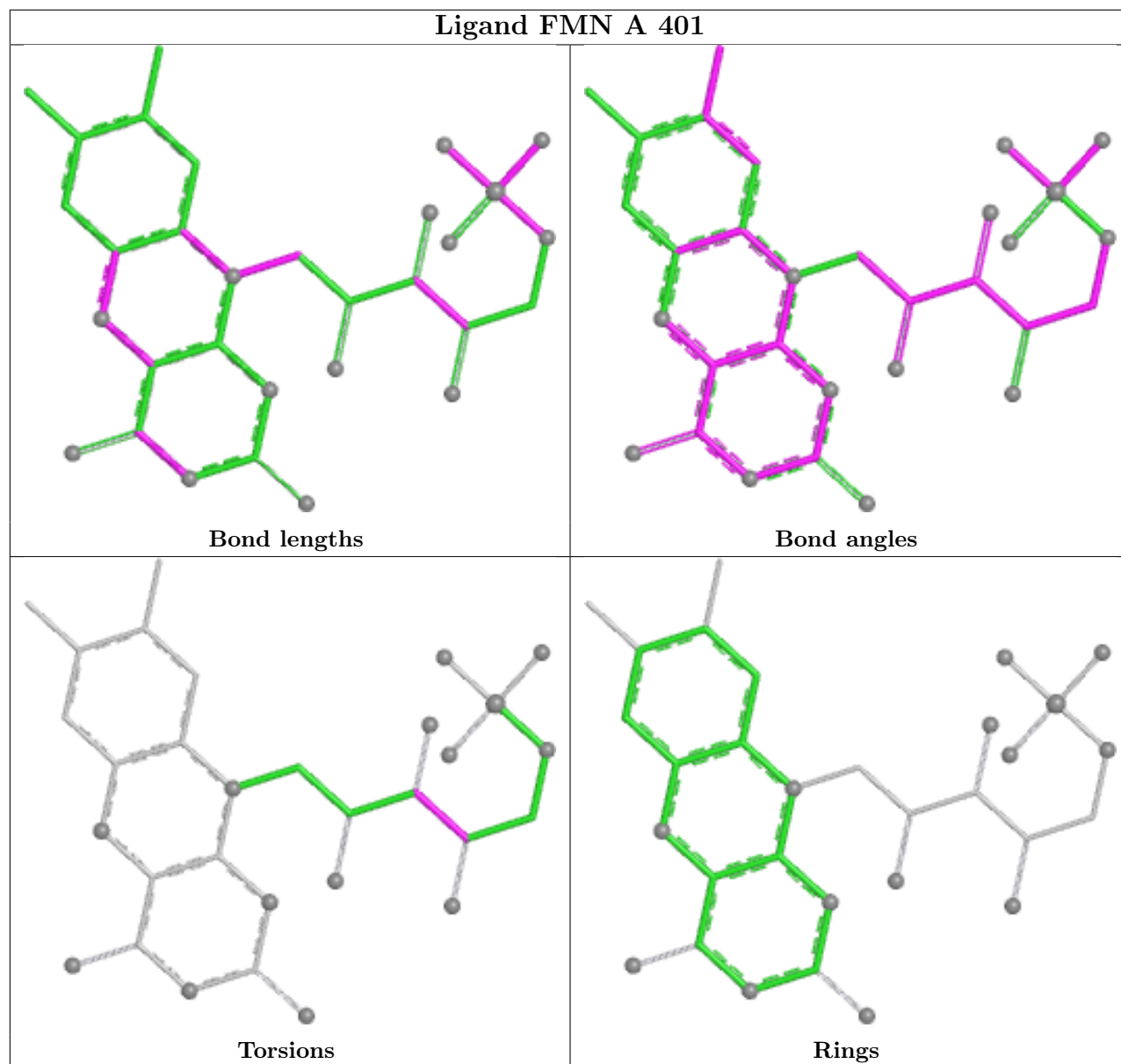
Mol	Chain	Res	Type	Atoms
2	A	401	FMN	C2'-C3'-C4'-O4'
2	A	401	FMN	O3'-C3'-C4'-C5'
2	A	401	FMN	C2'-C3'-C4'-C5'
2	A	401	FMN	O3'-C3'-C4'-O4'

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	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.