



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 06:04 PM UTC

PDB ID : 1OYB / pdb_00001oyb
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

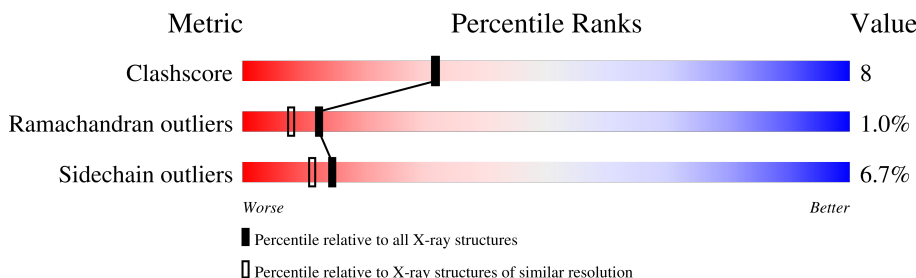
1 Overall quality at a glance

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	 62% 30% 6% •

2 Entry composition [i](#)

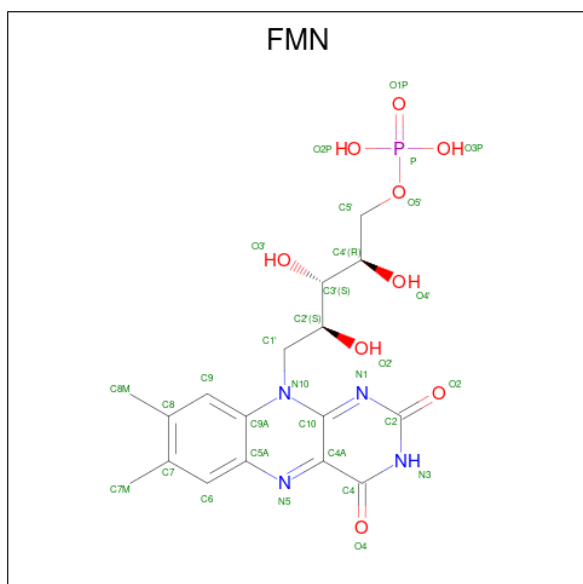
There are 4 unique types of molecules in this entry. The entry contains 4308 atoms, of which 964 are hydrogens and 0 are deuteriums.

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.

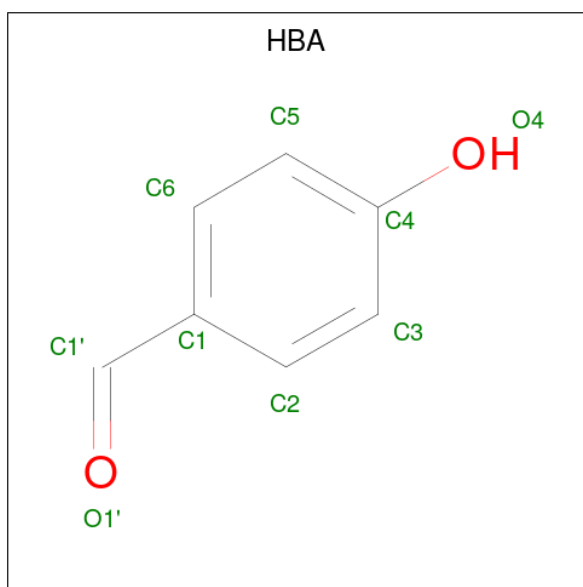
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	399	Total	C	H	N	O	S	4	0	0
			3886	2027	708	551	594	6			

- 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 P-HYDROXYBENZALDEHYDE (CCD ID: HBA) (formula: $C_7H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			9	7	2		

- Molecule 4 is water.

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

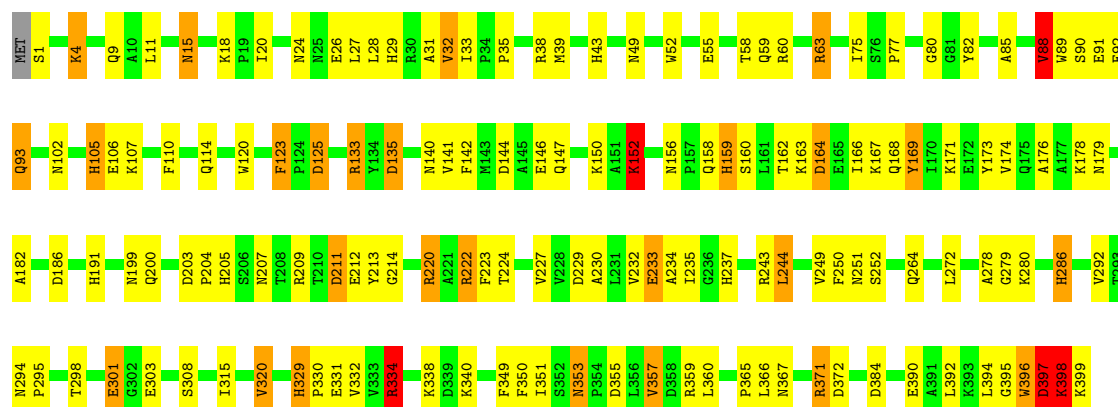
3 Residue-property plots

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: OLD YELLOW ENZYME

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	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}	0.173 , 0.236	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4308	wwPDB-VP
Average B, all atoms (Å ²)	16.0	wwPDB-VP

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: HBA, 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	1.40	20/3260 (0.6%)	2.11	123/4417 (2.8%)

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	4

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	329	HIS	CD2-NE2	-7.20	1.29	1.37
1	A	32	VAL	CA-CB	7.18	1.65	1.54
1	A	320	VAL	CA-CB	7.11	1.65	1.54
1	A	75	ILE	CA-CB	6.79	1.62	1.54
1	A	191	HIS	CD2-NE2	-6.78	1.30	1.37
1	A	38	ARG	CD-NE	-6.41	1.37	1.46
1	A	43	HIS	CD2-NE2	-6.15	1.31	1.37
1	A	237	HIS	CD2-NE2	-5.99	1.31	1.37
1	A	159	HIS	CD2-NE2	-5.95	1.31	1.37
1	A	205	HIS	CD2-NE2	-5.93	1.31	1.37
1	A	250	PHE	CA-CB	-5.86	1.43	1.53
1	A	29	HIS	CD2-NE2	-5.84	1.31	1.37
1	A	397	ASP	CA-C	-5.74	1.45	1.52
1	A	105	HIS	CD2-NE2	-5.73	1.31	1.37
1	A	29	HIS	CG-ND1	-5.68	1.31	1.38
1	A	292	VAL	CA-CB	5.67	1.62	1.54
1	A	35	PRO	CA-CB	-5.26	1.46	1.53
1	A	20	ILE	CA-CB	5.24	1.61	1.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	80	GLY	CA-C	-5.13	1.46	1.51
1	A	220	ARG	CD-NE	-5.04	1.39	1.46

All (123) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	38	ARG	NE-CZ-NH2	-11.82	108.56	119.20
1	A	233	GLU	CB-CG-CD	10.78	130.92	112.60
1	A	93	GLN	OE1-CD-NE2	-10.65	111.95	122.60
1	A	207	ASN	OD1-CG-ND2	-10.44	112.16	122.60
1	A	179	ASN	OD1-CG-ND2	-9.62	112.98	122.60
1	A	220	ARG	NE-CZ-NH2	-9.48	110.66	119.20
1	A	38	ARG	CG-CD-NE	-9.11	91.96	112.00
1	A	38	ARG	NE-CZ-NH1	9.09	130.59	121.50
1	A	200	GLN	OE1-CD-NE2	-8.93	113.67	122.60
1	A	164	ASP	CA-CB-CG	-8.78	103.82	112.60
1	A	88	VAL	N-CA-CB	-8.66	96.93	111.23
1	A	264	GLN	CG-CD-NE2	8.45	129.07	116.40
1	A	353	ASN	OD1-CG-ND2	-8.34	114.26	122.60
1	A	147	GLN	N-CA-C	-8.33	101.44	111.69
1	A	140	ASN	OD1-CG-ND2	-8.33	114.27	122.60
1	A	349	PHE	CA-CB-CG	-8.20	105.60	113.80
1	A	232	VAL	CA-C-O	-8.18	111.97	121.05
1	A	264	GLN	OE1-CD-NE2	-7.97	114.63	122.60
1	A	159	HIS	CB-CG-CD2	-7.75	121.13	131.20
1	A	398	LYS	N-CA-C	-7.64	94.53	110.80
1	A	397	ASP	CA-CB-CG	-7.63	104.97	112.60
1	A	353	ASN	CA-CB-CG	7.52	120.12	112.60
1	A	110	PHE	CA-CB-CG	-7.41	106.39	113.80
1	A	85	ALA	N-CA-C	-7.33	99.92	110.40
1	A	169	TYR	N-CA-C	-7.31	103.34	111.82
1	A	105	HIS	CB-CG-CD2	-7.30	121.71	131.20
1	A	144	ASP	CA-CB-CG	7.25	119.86	112.60
1	A	249	VAL	N-CA-C	-7.20	106.20	113.47
1	A	280	LYS	N-CA-C	7.15	119.79	109.71
1	A	15	ASN	OD1-CG-ND2	-7.14	115.46	122.60
1	A	49	ASN	CA-CB-CG	-7.13	105.47	112.60
1	A	179	ASN	CB-CG-ND2	7.04	126.95	116.40
1	A	222	ARG	CG-CD-NE	-7.03	96.53	112.00
1	A	301	GLU	CA-CB-CG	-7.03	100.04	114.10
1	A	166	ILE	N-CA-C	-6.89	104.05	110.53
1	A	396	TRP	CA-C-N	6.87	134.66	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	396	TRP	C-N-CA	6.87	134.66	121.54
1	A	158	GLN	OE1-CD-NE2	-6.84	115.76	122.60
1	A	160	SER	CA-CB-OG	-6.84	97.42	111.10
1	A	142	PHE	CA-CB-CG	-6.80	107.00	113.80
1	A	233	GLU	CA-CB-CG	6.78	127.65	114.10
1	A	397	ASP	O-C-N	6.70	131.50	122.59
1	A	220	ARG	NE-CZ-NH1	6.52	128.02	121.50
1	A	152	LYS	CA-C-O	-6.49	113.54	120.42
1	A	223	PHE	CA-CB-CG	6.45	120.25	113.80
1	A	63	ARG	CA-C-N	6.44	126.47	119.90
1	A	63	ARG	C-N-CA	6.44	126.47	119.90
1	A	49	ASN	OD1-CG-ND2	-6.43	116.17	122.60
1	A	182	ALA	O-C-N	-6.42	115.32	122.12
1	A	159	HIS	CB-CG-ND1	6.41	132.31	122.70
1	A	191	HIS	CB-CG-CD2	-6.40	122.88	131.20
1	A	351	ILE	CA-C-O	-6.32	114.52	121.29
1	A	178	LYS	CA-CB-CG	-6.32	101.46	114.10
1	A	229	ASP	N-CA-C	6.23	118.15	111.36
1	A	93	GLN	CG-CD-NE2	6.20	125.69	116.40
1	A	280	LYS	CA-CB-CG	-6.18	101.74	114.10
1	A	135	ASP	N-CA-C	6.18	120.12	110.17
1	A	220	ARG	CB-CG-CD	-6.18	97.09	111.30
1	A	120	TRP	CA-CB-CG	6.16	125.31	113.60
1	A	205	HIS	CB-CG-CD2	-6.15	123.20	131.20
1	A	207	ASN	CB-CG-ND2	6.11	125.56	116.40
1	A	102	ASN	CB-CG-ND2	6.09	125.54	116.40
1	A	4	LYS	N-CA-C	6.01	123.61	110.80
1	A	303	GLU	N-CA-CB	-6.01	100.99	110.06
1	A	58	THR	N-CA-C	-6.00	104.65	111.07
1	A	355	ASP	CA-CB-CG	5.96	118.56	112.60
1	A	294	ASN	OD1-CG-ND2	-5.96	116.64	122.60
1	A	24	ASN	OD1-CG-ND2	-5.93	116.67	122.60
1	A	147	GLN	OE1-CD-NE2	-5.93	116.67	122.60
1	A	33	ILE	N-CA-C	-5.87	102.22	107.56
1	A	279	GLY	O-C-N	-5.87	115.24	122.46
1	A	88	VAL	CB-CA-C	5.86	120.90	111.29
1	A	38	ARG	CD-NE-CZ	5.85	132.59	124.40
1	A	125	ASP	CA-CB-CG	5.84	118.44	112.60
1	A	168	GLN	OE1-CD-NE2	-5.83	116.77	122.60
1	A	384	ASP	CA-CB-CG	5.78	118.38	112.60
1	A	133	ARG	NE-CZ-NH1	5.75	127.25	121.50
1	A	164	ASP	N-CA-C	5.73	117.20	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	123	PHE	O-C-N	-5.73	116.44	121.31
1	A	52	TRP	CG-CD2-CE3	5.71	139.62	133.90
1	A	179	ASN	CA-CB-CG	5.68	118.28	112.60
1	A	191	HIS	CB-CG-ND1	5.67	131.21	122.70
1	A	211	ASP	CA-CB-CG	5.67	118.27	112.60
1	A	159	HIS	CA-C-O	-5.65	114.72	120.71
1	A	237	HIS	CB-CG-CD2	-5.57	123.95	131.20
1	A	156	ASN	OD1-CG-ND2	-5.54	117.06	122.60
1	A	334	ARG	CG-CD-NE	-5.52	99.85	112.00
1	A	31	ALA	CA-C-O	-5.52	114.80	120.54
1	A	133	ARG	CB-CG-CD	-5.51	98.63	111.30
1	A	199	ASN	OD1-CG-ND2	-5.50	117.10	122.60
1	A	162	THR	N-CA-C	-5.49	102.62	110.59
1	A	227	VAL	O-C-N	-5.49	116.53	121.91
1	A	39	MET	N-CA-C	5.48	118.99	111.54
1	A	105	HIS	CB-CG-ND1	5.43	130.85	122.70
1	A	338	LYS	N-CA-C	-5.43	105.46	111.71
1	A	4	LYS	CA-C-N	-5.40	114.52	122.83
1	A	4	LYS	C-N-CA	-5.40	114.52	122.83
1	A	60	ARG	CA-CB-CG	-5.38	103.34	114.10
1	A	332	VAL	O-C-N	-5.37	116.31	121.90
1	A	31	ALA	N-CA-C	-5.37	99.01	108.20
1	A	315	ILE	CB-CG1-CD1	-5.30	102.66	113.80
1	A	224	THR	CA-CB-OG1	-5.30	101.65	109.60
1	A	199	ASN	CB-CG-ND2	5.29	124.34	116.40
1	A	357	VAL	CA-C-O	-5.29	115.45	120.95
1	A	235	ILE	N-CA-C	5.26	118.25	113.20
1	A	372	ASP	CA-CB-CG	-5.25	107.35	112.60
1	A	286	HIS	CB-CG-ND1	5.25	130.57	122.70
1	A	334	ARG	NE-CZ-NH1	5.24	126.74	121.50
1	A	4	LYS	CA-C-O	-5.21	113.05	120.51
1	A	338	LYS	CG-CD-CE	-5.17	99.42	111.30
1	A	135	ASP	O-C-N	-5.16	117.16	123.10
1	A	244	LEU	O-C-N	-5.16	116.98	123.27
1	A	330	PRO	N-CA-C	-5.15	107.42	113.86
1	A	91	GLU	CB-CA-C	-5.14	102.25	110.79
1	A	102	ASN	OD1-CG-ND2	-5.14	117.46	122.60
1	A	173	TYR	O-C-N	-5.11	116.81	122.07
1	A	252	SER	N-CA-C	5.10	118.75	111.92
1	A	123	PHE	CA-C-O	-5.08	115.55	119.46
1	A	133	ARG	NE-CZ-NH2	-5.03	114.67	119.20
1	A	179	ASN	N-CA-C	5.03	116.76	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	251	ASN	OD1-CG-ND2	-5.02	117.58	122.60
1	A	27	LEU	N-CA-C	-5.00	103.07	110.48
1	A	167	LYS	N-CA-C	5.00	116.73	111.28

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	169	TYR	Sidechain
1	A	220	ARG	Sidechain
1	A	397	ASP	Mainchain
1	A	82	TYR	Sidechain

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	50	0
2	A	31	4	19	1	0
3	A	9	0	5	1	0
4	A	126	252	0	4	0
All	All	3344	964	3117	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 8.

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:114:GLN:HE22	2:A:401:FMN:HN3	1.24	0.81
3:A:402:HBA:H5	4:A:616:HOH:O	1.86	0.75
1:A:353:ASN:HD21	1:A:367:ASN:H	1.38	0.71
1:A:295:PRO:HG3	4:A:616:HOH:O	1.90	0.70
1:A:398:LYS:HZ3	1:A:399:LYS:H	1.44	0.65
1:A:163:LYS:HZ1	1:A:212:GLU:HG3	1.65	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63:ARG:HG2	1:A:357:VAL:HG11	1.84	0.60
1:A:133:ARG:HD2	1:A:135:ASP:OD1	2.01	0.59
1:A:397:ASP:O	1:A:398:LYS:HB2	2.03	0.59
1:A:395:GLY:C	1:A:397:ASP:H	2.11	0.58
1:A:392:LEU:HD22	1:A:398:LYS:HB3	1.86	0.57
1:A:392:LEU:O	1:A:399:LYS:HA	2.04	0.57
1:A:90:SER:H	1:A:93:GLN:NE2	2.03	0.57
1:A:92:GLU:HG3	4:A:635:HOH:O	2.06	0.54
1:A:105:HIS:HE1	1:A:186:ASP:OD2	1.90	0.54
1:A:230:ALA:O	1:A:233:GLU:HG3	2.08	0.53
1:A:298:THR:O	1:A:301:GLU:HB2	2.09	0.53
1:A:63:ARG:HD2	4:A:583:HOH:O	2.08	0.53
1:A:9:GLN:NE2	1:A:334:ARG:HH11	2.08	0.52
1:A:89:TRP:H	1:A:93:GLN:HE22	1.56	0.51
1:A:88:VAL:HG13	1:A:176:ALA:HB1	1.92	0.51
1:A:89:TRP:H	1:A:93:GLN:NE2	2.10	0.50
1:A:353:ASN:ND2	1:A:367:ASN:H	2.09	0.50
1:A:55:GLU:O	1:A:59:GLN:HG3	2.13	0.48
1:A:395:GLY:O	1:A:397:ASP:N	2.46	0.48
1:A:398:LYS:HZ3	1:A:399:LYS:N	2.11	0.48
1:A:243:ARG:HH21	1:A:286:HIS:CE1	2.30	0.48
1:A:15:ASN:HA	1:A:18:LYS:HD3	1.97	0.46
1:A:398:LYS:NZ	1:A:399:LYS:N	2.64	0.45
1:A:77:PRO:HD3	1:A:89:TRP:CE2	2.51	0.45
1:A:353:ASN:HD21	1:A:367:ASN:N	2.11	0.45
1:A:123:PHE:HB3	1:A:125:ASP:OD1	2.18	0.44
1:A:174:VAL:HG13	1:A:234:ALA:HB2	1.99	0.44
1:A:390:GLU:O	1:A:394:LEU:HG	2.18	0.44
1:A:9:GLN:HE21	1:A:334:ARG:HH11	1.63	0.43
1:A:329:HIS:HD2	1:A:331:GLU:OE2	2.02	0.43
1:A:163:LYS:HE3	1:A:211:ASP:OD2	2.19	0.43
1:A:133:ARG:HD3	1:A:159:HIS:CD2	2.53	0.42
1:A:4:LYS:HA	1:A:4:LYS:HD3	1.88	0.42
1:A:163:LYS:NZ	1:A:212:GLU:HG3	2.31	0.42
1:A:213:TYR:CE1	1:A:222:ARG:HG2	2.55	0.42
1:A:88:VAL:CG1	1:A:176:ALA:HB1	2.50	0.41
1:A:209:ARG:HB2	1:A:214:GLY:HA3	2.02	0.41
1:A:146:GLU:O	1:A:150:LYS:HG3	2.21	0.41
1:A:152:LYS:HD2	1:A:152:LYS:HA	1.47	0.41
1:A:203:ASP:HA	1:A:204:PRO:HD2	1.98	0.41
1:A:359:ARG:HD3	1:A:365:PRO:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:371:ARG:CZ	1:A:371:ARG:H	2.33	0.41
1:A:107:LYS:HD3	1:A:107:LYS:HA	1.91	0.41
1:A:163:LYS:NZ	1:A:211:ASP:HB2	2.36	0.41
1:A:398:LYS:NZ	1:A:399:LYS:H	2.14	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%)	377 (95%)	16 (4%)	4 (1%)	12 8

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	398	LYS
1	A	278	ALA
1	A	396	TRP
1	A	397	ASP

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%)	306 (93%)	22 (7%)	15 11

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	SER
1	A	11	LEU
1	A	26	GLU
1	A	28	LEU
1	A	32	VAL
1	A	88	VAL
1	A	106	GLU
1	A	141	VAL
1	A	152	LYS
1	A	164	ASP
1	A	171	LYS
1	A	244	LEU
1	A	272	LEU
1	A	308	SER
1	A	320	VAL
1	A	334	ARG
1	A	340	LYS
1	A	350	PHE
1	A	360	LEU
1	A	366	LEU
1	A	371	ARG
1	A	398	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) 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	114	GLN
1	A	147	GLN
1	A	156	ASN
1	A	168	GLN
1	A	200	GLN
1	A	286	HIS
1	A	329	HIS
1	A	353	ASN
1	A	367	ASN
1	A	380	HIS

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$
3	HBA	A	402	-	9,9,9	2.12	2 (22%)	11,11,11	1.26	1 (9%)
2	FMN	A	401	-	33,33,33	1.43	7 (21%)	48,50,50	1.18	4 (8%)

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
3	HBA	A	402	-	-	0/2/2/2	0/1/1/1
2	FMN	A	401	-	-	1/18/18/18	0/3/3/3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	402	HBA	O4-C4	-5.30	1.25	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	FMN	C5A-N5	-2.99	1.33	1.39
3	A	402	HBA	C1-C1'	-2.84	1.39	1.47
2	A	401	FMN	C1'-C2'	2.55	1.56	1.52
2	A	401	FMN	C10-N1	2.39	1.38	1.33
2	A	401	FMN	P-O2P	-2.38	1.46	1.54
2	A	401	FMN	C4A-N5	2.38	1.35	1.30
2	A	401	FMN	P-O5'	-2.21	1.53	1.60
2	A	401	FMN	C8-C7	2.20	1.46	1.40

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	FMN	C4-C4A-N5	2.61	121.81	118.21
2	A	401	FMN	C6-C5A-C9A	2.38	122.31	119.05
2	A	401	FMN	O2P-P-O1P	2.27	119.67	110.83
2	A	401	FMN	O3P-P-O5'	-2.16	101.05	106.67
3	A	402	HBA	O1'-C1'-C1	-2.12	117.37	124.56

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	FMN	C4'-C5'-O5'-P

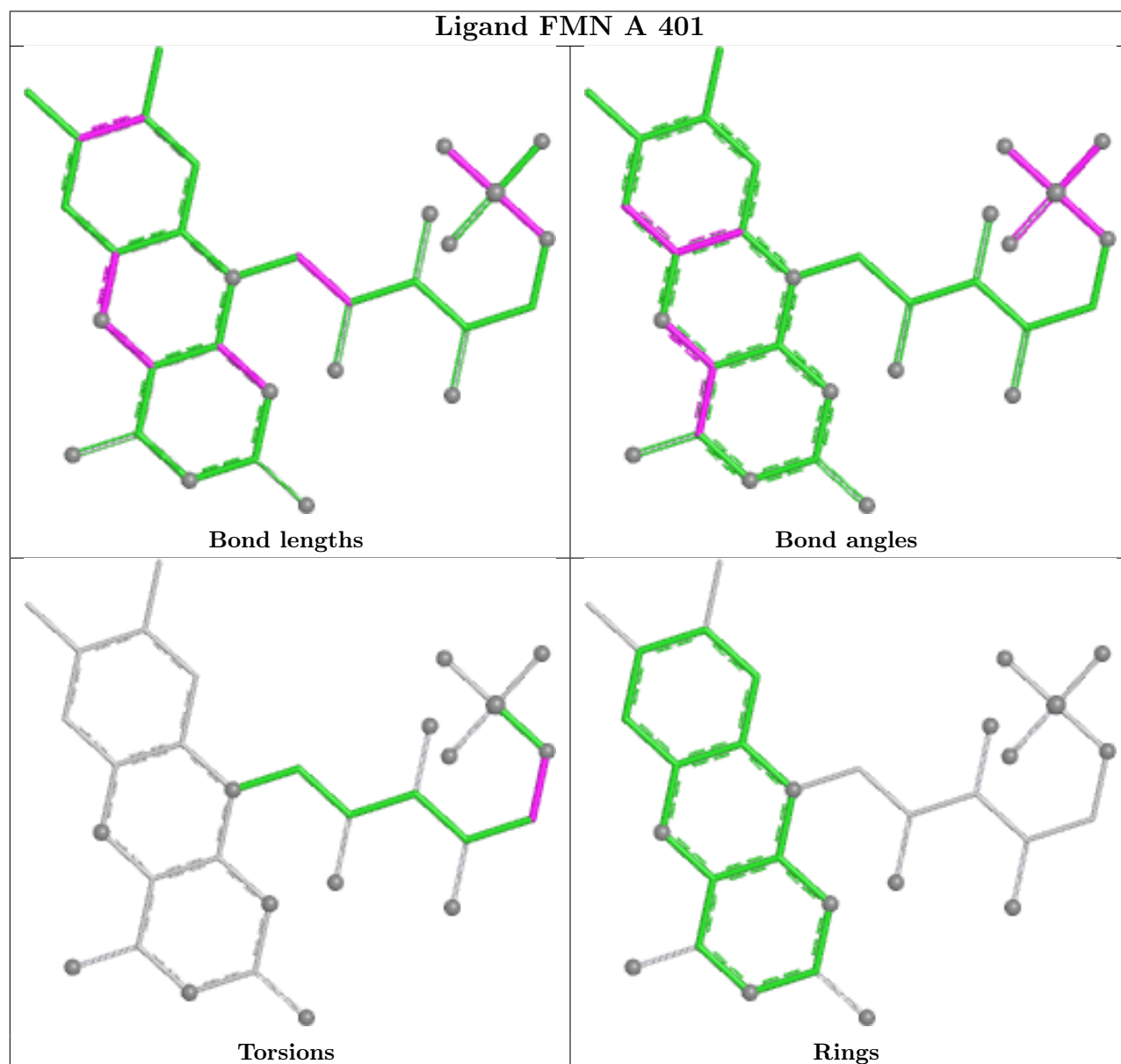
There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	402	HBA	1	0
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.