Full wwPDB X-ray Structure Validation Report ⓘ

Feb 4, 2024 – 08:00 AM EST

PDB ID	:	1OYC
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:

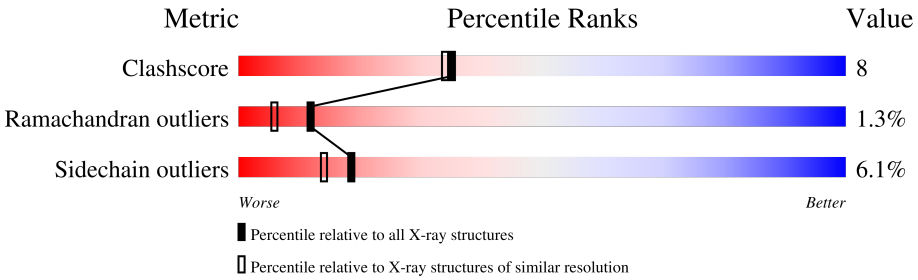
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	400	68% 25% 6% ·

2 Entry composition

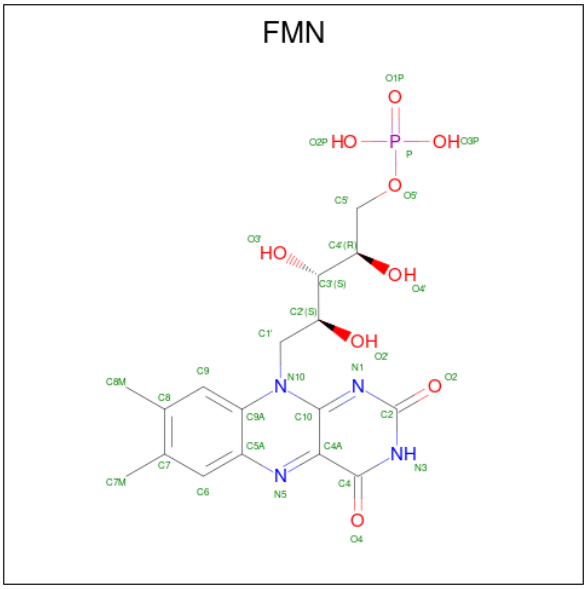
There are 3 unique types of molecules in this entry. The entry contains 4299 atoms, of which 964 are hydrogens and 0 are deuteriums.

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
			Total	C	H	N	O	S			
1	A	399	3886	2027	708	551	594	6	4	0	0

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



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

- Molecule 3 is water.

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

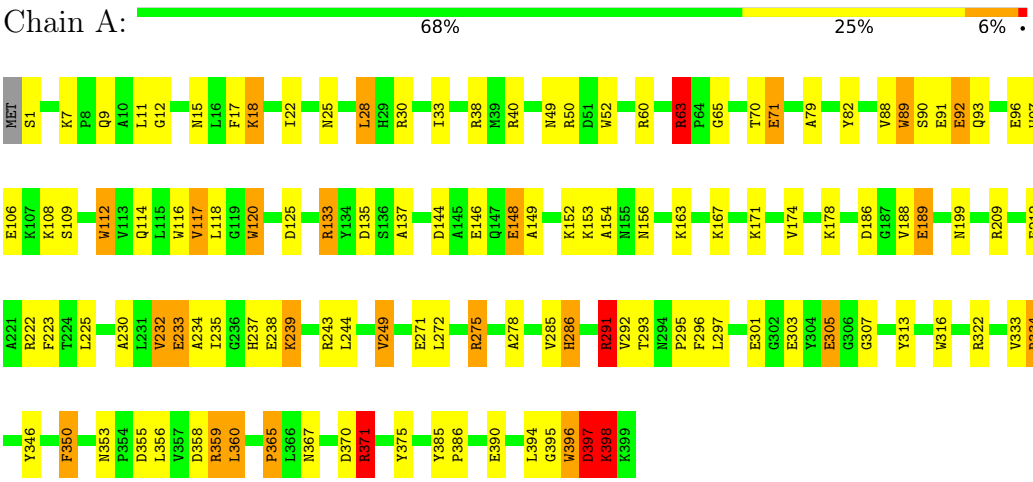
3 Residue-property plots (i)

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

Chain A:



4 Data and refinement statistics (i)

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	1.24	6/3260 (0.2%)	2.03	97/4417 (2.2%)

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 (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	88	VAL	CB-CG2	-5.83	1.40	1.52
1	A	189	GLU	CD-OE2	-5.58	1.19	1.25
1	A	97	TRP	CG-CD2	-5.16	1.34	1.43
1	A	71	GLU	CB-CG	-5.13	1.42	1.52
1	A	305	GLU	CB-CG	5.07	1.61	1.52
1	A	109	SER	CA-CB	-5.01	1.45	1.52

All (97) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	220	ARG	NE-CZ-NH1	17.56	129.08	120.30
1	A	38	ARG	NE-CZ-NH2	-17.16	111.72	120.30
1	A	291	ARG	NE-CZ-NH1	15.86	128.23	120.30
1	A	220	ARG	NE-CZ-NH2	-15.23	112.68	120.30
1	A	133	ARG	NE-CZ-NH2	-14.88	112.86	120.30
1	A	30	ARG	NE-CZ-NH1	14.04	127.32	120.30
1	A	334	ARG	NE-CZ-NH1	13.99	127.29	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	334	ARG	NE-CZ-NH2	-13.55	113.53	120.30
1	A	397	ASP	CA-C-N	-13.53	87.43	117.20
1	A	133	ARG	NE-CZ-NH1	12.61	126.61	120.30
1	A	38	ARG	CG-CD-NE	-12.16	86.27	111.80
1	A	38	ARG	NE-CZ-NH1	10.15	125.37	120.30
1	A	82	TYR	CB-CG-CD2	-9.71	115.17	121.00
1	A	275	ARG	NE-CZ-NH2	-9.66	115.47	120.30
1	A	371	ARG	CA-CB-CG	9.66	134.65	113.40
1	A	52	TRP	CD1-CG-CD2	9.60	113.98	106.30
1	A	30	ARG	NE-CZ-NH2	-9.04	115.78	120.30
1	A	63	ARG	NE-CZ-NH1	8.91	124.75	120.30
1	A	385	TYR	CB-CG-CD1	-8.73	115.76	121.00
1	A	275	ARG	NE-CZ-NH1	8.56	124.58	120.30
1	A	52	TRP	CE2-CD2-CG	-8.49	100.50	107.30
1	A	146	GLU	CA-CB-CG	8.34	131.75	113.40
1	A	52	TRP	CG-CD2-CE3	7.85	140.97	133.90
1	A	82	TYR	CB-CG-CD1	7.81	125.69	121.00
1	A	116	TRP	CD1-CG-CD2	7.61	112.39	106.30
1	A	316	TRP	CE2-CD2-CG	-7.58	101.23	107.30
1	A	88	VAL	CG1-CB-CG2	7.57	123.01	110.90
1	A	18	LYS	CA-CB-CG	-7.56	96.78	113.40
1	A	106	GLU	CA-CB-CG	7.46	129.81	113.40
1	A	249	VAL	CG1-CB-CG2	-7.38	99.09	110.90
1	A	359	ARG	NE-CZ-NH1	7.36	123.98	120.30
1	A	232	VAL	CG1-CB-CG2	-7.16	99.45	110.90
1	A	291	ARG	NH1-CZ-NH2	-7.16	111.53	119.40
1	A	89	TRP	CE2-CD2-CG	-7.14	101.59	107.30
1	A	239	LYS	CA-CB-CG	-7.14	97.69	113.40
1	A	371	ARG	NE-CZ-NH2	-7.13	116.74	120.30
1	A	52	TRP	CB-CG-CD1	-7.02	117.87	127.00
1	A	322	ARG	NE-CZ-NH1	7.02	123.81	120.30
1	A	209	ARG	NE-CZ-NH2	6.93	123.77	120.30
1	A	375	TYR	CB-CG-CD2	-6.88	116.87	121.00
1	A	316	TRP	CD1-CG-CD2	6.75	111.70	106.30
1	A	178	LYS	CA-CB-CG	-6.70	98.67	113.40
1	A	285	VAL	CG1-CB-CG2	-6.67	100.23	110.90
1	A	370	ASP	CB-CG-OD1	6.55	124.19	118.30
1	A	63	ARG	NE-CZ-NH2	-6.50	117.05	120.30
1	A	88	VAL	N-CA-CB	-6.36	97.52	111.50
1	A	50	ARG	NE-CZ-NH2	-6.35	117.12	120.30
1	A	396	TRP	CG-CD2-CE3	6.34	139.60	133.90
1	A	89	TRP	CG-CD2-CE3	6.32	139.59	133.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	91	GLU	CA-CB-CG	6.23	127.10	113.40
1	A	154	ALA	CB-CA-C	-6.17	100.84	110.10
1	A	112	TRP	CD1-CG-CD2	6.17	111.23	106.30
1	A	220	ARG	CG-CD-NE	-6.13	98.92	111.80
1	A	370	ASP	CB-CG-OD2	-6.12	112.80	118.30
1	A	97	TRP	CE2-CD2-CG	-6.10	102.42	107.30
1	A	89	TRP	CD1-CG-CD2	6.07	111.16	106.30
1	A	125	ASP	CB-CG-OD1	6.03	123.73	118.30
1	A	396	TRP	CE2-CD2-CG	-6.03	102.48	107.30
1	A	52	TRP	CG-CD1-NE1	-6.01	104.09	110.10
1	A	316	TRP	CG-CD2-CE3	5.97	139.27	133.90
1	A	116	TRP	CE2-CD2-CG	-5.76	102.69	107.30
1	A	117	VAL	CG1-CB-CG2	-5.72	101.75	110.90
1	A	116	TRP	CG-CD1-NE1	-5.67	104.43	110.10
1	A	398	LYS	N-CA-C	-5.66	95.71	111.00
1	A	137	ALA	CB-CA-C	-5.58	101.73	110.10
1	A	218	GLU	CA-CB-CG	5.57	125.65	113.40
1	A	144	ASP	CA-CB-CG	5.56	125.64	113.40
1	A	60	ARG	CA-CB-CG	-5.55	101.18	113.40
1	A	148	GLU	N-CA-CB	-5.55	100.61	110.60
1	A	97	TRP	CD1-CG-CD2	5.55	110.74	106.30
1	A	358	ASP	CB-CG-OD1	5.54	123.28	118.30
1	A	89	TRP	CB-CG-CD1	-5.51	119.83	127.00
1	A	220	ARG	CB-CG-CD	-5.51	97.27	111.60
1	A	112	TRP	CE2-CD2-CG	-5.51	102.89	107.30
1	A	316	TRP	CB-CG-CD1	-5.50	119.84	127.00
1	A	225	LEU	CA-C-N	5.50	129.30	117.20
1	A	96	GLU	CA-C-N	5.50	129.29	117.20
1	A	108	LYS	CB-CG-CD	-5.48	97.35	111.60
1	A	88	VAL	CB-CA-C	5.43	121.71	111.40
1	A	396	TRP	CA-C-N	-5.41	105.30	117.20
1	A	118	LEU	CA-C-N	5.41	127.01	116.20
1	A	71	GLU	CB-CA-C	-5.35	99.71	110.40
1	A	307	GLY	CA-C-N	-5.34	105.44	117.20
1	A	296	PHE	CA-CB-CG	-5.34	101.09	113.90
1	A	396	TRP	CD1-CG-CD2	5.28	110.53	106.30
1	A	233	GLU	CB-CG-CD	5.27	128.44	114.20
1	A	102	ASN	CB-CG-ND2	5.26	129.34	116.70
1	A	249	VAL	O-C-N	-5.22	114.35	122.70
1	A	249	VAL	CA-C-N	5.20	128.63	117.20
1	A	120	TRP	CE2-CD2-CG	-5.18	103.15	107.30
1	A	70	THR	OG1-CB-CG2	-5.15	98.14	110.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	92	GLU	CA-CB-CG	5.13	124.69	113.40
1	A	225	LEU	O-C-N	-5.12	114.50	122.70
1	A	96	GLU	O-C-N	-5.12	114.51	122.70
1	A	355	ASP	CB-CG-OD1	5.11	122.90	118.30
1	A	375	TYR	O-C-N	-5.09	114.55	122.70
1	A	188	VAL	CG1-CB-CG2	-5.09	102.76	110.90

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 (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	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:398:LYS:HZ2	1:A:398:LYS:HB3	1.80	0.47
1:A:189:GLU:OE2	1:A:286:HIS:HD2	1.98	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:395:GLY:C	1:A:397:ASP:H	2.24	0.40
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
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%)	12 6

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%)	308 (94%)	20 (6%)	18 14

All (20) 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	63	ARG
1	A	120	TRP
1	A	156	ASN
1	A	199	ASN
1	A	223	PHE
1	A	238	GLU
1	A	244	LEU
1	A	272	LEU
1	A	286	HIS
1	A	291	ARG
1	A	340	LYS
1	A	350	PHE
1	A	360	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 (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	GLN
1	A	25	ASN
1	A	93	GLN
1	A	105	HIS
1	A	114	GLN
1	A	126	ASN
1	A	147	GLN
1	A	156	ASN
1	A	175	GLN
1	A	179	ASN
1	A	191	HIS
1	A	200	GLN
1	A	286	HIS

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Mol	Chain	Res	Type
1	A	353	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 monosaccharides 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	401	-	33,33,33	1.60	9 (27%)	48,50,50	2.37	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	4.01	1.38	1.30
2	A	401	FMN	P-O2P	-2.80	1.44	1.54
2	A	401	FMN	C4'-C3'	-2.70	1.48	1.53
2	A	401	FMN	P-O1P	-2.44	1.42	1.50
2	A	401	FMN	P-O5'	-2.26	1.52	1.60
2	A	401	FMN	C4-N3	2.17	1.42	1.38
2	A	401	FMN	C5A-N5	-2.07	1.35	1.39
2	A	401	FMN	C1'-N10	2.05	1.53	1.48
2	A	401	FMN	C9A-N10	-2.01	1.37	1.41

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	401	FMN	C5'-C4'-C3'	-9.91	93.06	112.20
2	A	401	FMN	C4-N3-C2	-3.99	118.28	125.64
2	A	401	FMN	C4-C4A-N5	3.91	123.79	118.23
2	A	401	FMN	O5'-C5'-C4'	-3.53	99.93	109.36
2	A	401	FMN	C10-N1-C2	3.46	123.83	116.90
2	A	401	FMN	O3'-C3'-C4'	-3.22	101.03	108.81
2	A	401	FMN	C5A-C9A-N10	2.99	121.05	117.95
2	A	401	FMN	O3'-C3'-C2'	2.94	115.92	108.81
2	A	401	FMN	C10-C4A-N5	-2.91	118.69	124.86
2	A	401	FMN	O4-C4-N3	-2.75	114.84	120.12
2	A	401	FMN	O2P-P-O1P	2.70	121.24	110.68
2	A	401	FMN	C8M-C8-C9	-2.54	114.80	119.49
2	A	401	FMN	O2'-C2'-C3'	-2.47	103.08	109.10
2	A	401	FMN	C4A-C10-N10	2.42	120.02	116.48
2	A	401	FMN	C4A-C10-N1	-2.33	119.33	124.73
2	A	401	FMN	C1'-C2'-C3'	2.20	115.94	109.79
2	A	401	FMN	C4A-C4-N3	2.01	118.28	113.19

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	O3'-C3'-C4'-O4'
2	A	401	FMN	C2'-C3'-C4'-C5'

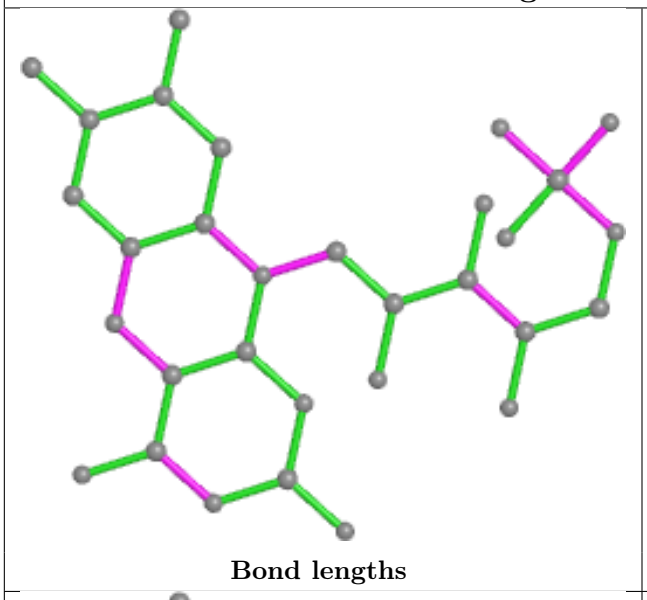
There are no ring outliers.

1 monomer is involved in 1 short contact:

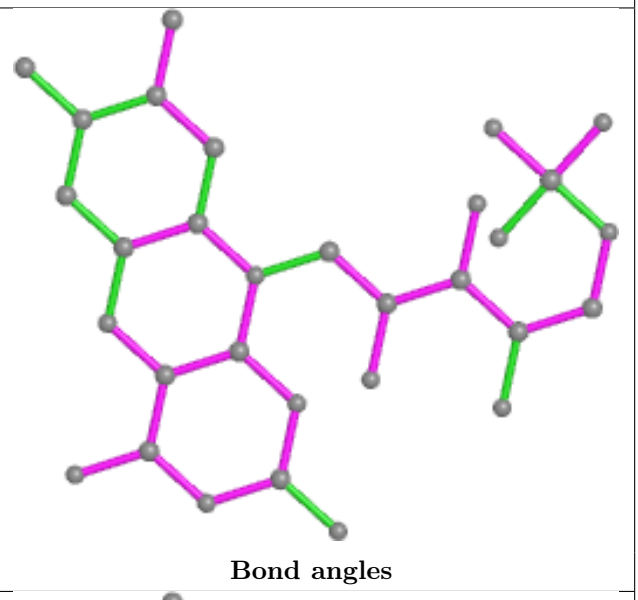
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	FMN	1	0

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 then 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.

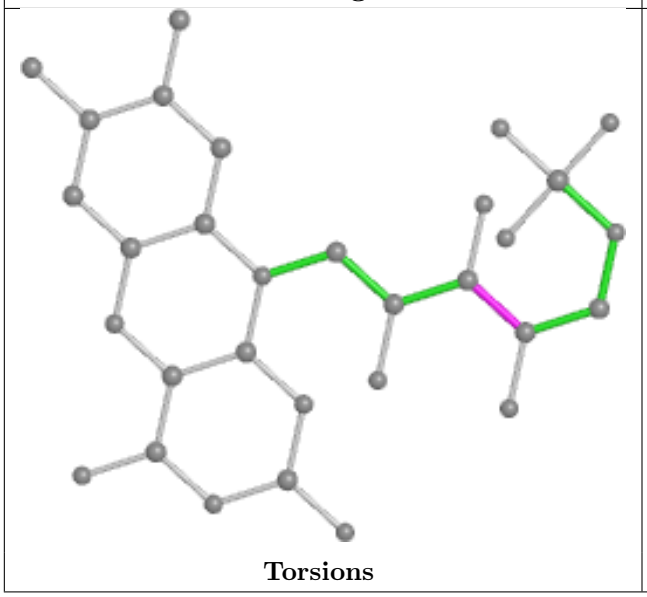
Ligand FMN A 401



Bond lengths



Bond angles



Torsions

Rings

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.