WORLDWIDE PDB PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Nov 21, 2023 – 06:18 AM JST

PDB ID	:	7F1Y
Title	:	L-lactate oxidase without substrate
Authors	:	Morimoto, Y.; Inaka, K.
Deposited on	:	2021-06-10
Resolution	:	1.33 Å(reported)

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)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
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 ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.33 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	Percentile Ranks	Value
Rfree		0.195
Clashscore		13
Ramachandran outliers		1.4%
Sidechain outliers		3.7%
RSRZ outliers		11.7%

Worse　　　　　　　　　　　　　　　　*Better*

▌ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
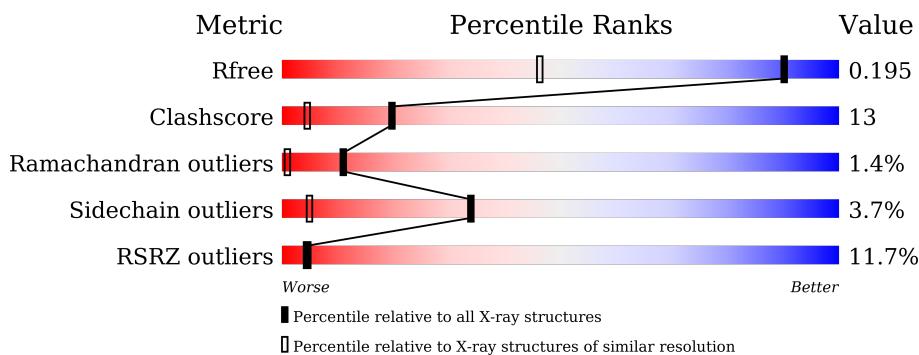
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1385 (1.36-1.32)
Clashscore	141614	1417 (1.36-1.32)
Ramachandran outliers	138981	1397 (1.36-1.32)
Sidechain outliers	138945	1397 (1.36-1.32)
RSRZ outliers	127900	1369 (1.36-1.32)

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% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	368	13%　　85%　　　　　　　　9%　· ·
1	B	368	10%　　77%　　　　　　　18%　· ·
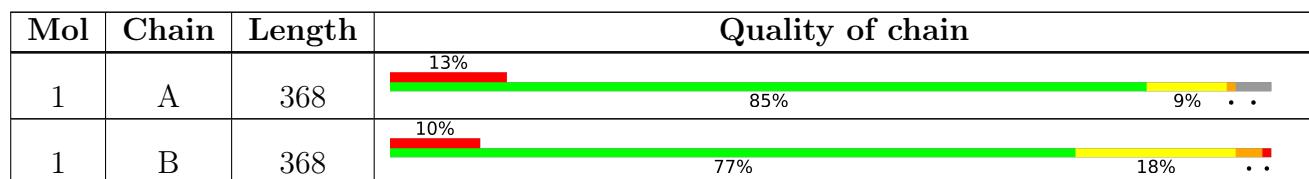
2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 6359 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 Lactate oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	352	Total 2717	C 1717	N 470	O 523	S 7	0	1	0
1	B	368	Total 2836	C 1792	N 491	O 546	S 7	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	232	ALA	GLY	conflict	UNP Q44467
B	232	ALA	GLY	conflict	UNP Q44467

- Molecule 2 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).

ACT

OXT

O^-

C

CH3—

O

O
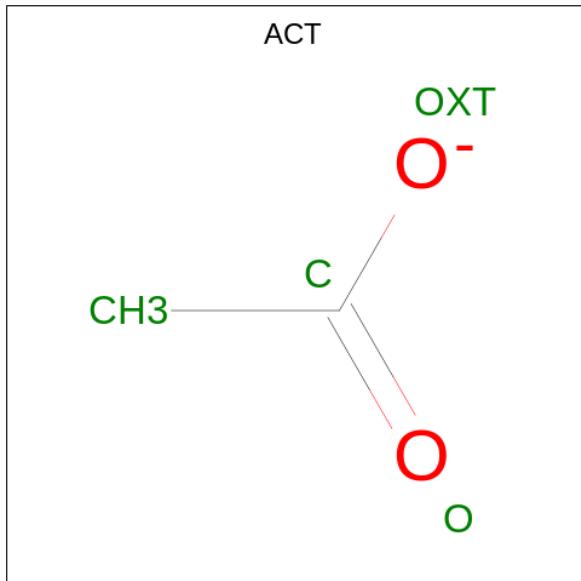
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total 4	C 2	O 2	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total 4	C 2	O 2	0	0

- Molecule 3 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: $C_{17}H_{21}N_4O_9P$) (labeled as "Ligand of Interest" by depositor).
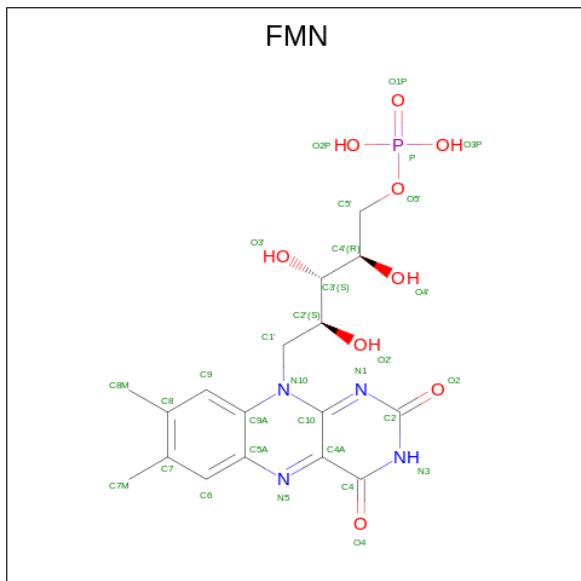
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 31	C 17	N 4	O 9	P 1	0	0
3	B	1	Total 31	C 17	N 4	O 9	P 1	0	0

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).

EDO

O2

OH

C1

C2

HO

O1
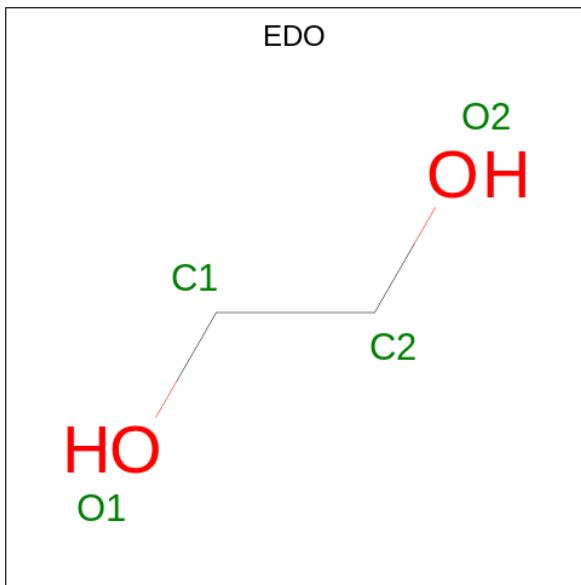
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total 4	C 2	O 2	0	0
4	B	1	Total 4	C 2	O 2	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	364	Total 364	O 364	0	0
5	B	364	Total 364	O 364	0	0

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 and electron density. 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. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). 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.

• Molecule 1: Lactate oxidase

Chain A:

• Molecule 1: Lactate oxidase

Chain B:
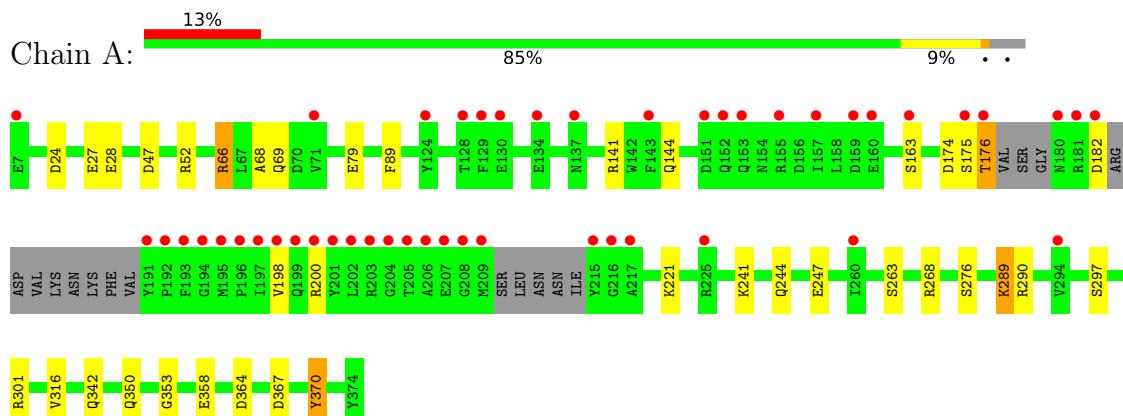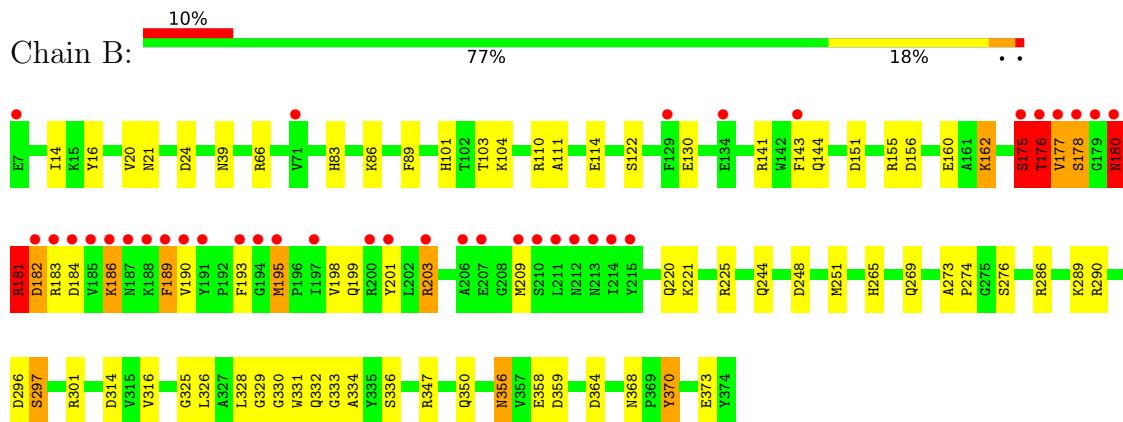
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	I 4	Depositor
Cell constants a, b, c, α, β, γ	132.30Å 132.30Å 91.23Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.66 – 1.33 45.62 – 1.33	Depositor EDS
% Data completeness (in resolution range)	98.4 (45.66-1.33) 98.4 (45.62-1.33)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.25 (at 1.33Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.170 , 0.193 0.173 , 0.195	Depositor DCC
R_{free} test set	8622 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å^2)	17.4	Xtriage
Anisotropy	0.089	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 44.4	EDS
L-test for twinning [2]	$< |L| > = 0.50, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.013 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	6359	wwPDB-VP
Average B, all atoms (Å^2)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.26% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1] Intensities estimated from amplitudes.
[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5　Model quality ⓘ

5.1　Standard geometry ⓘ

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

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	0.79	1/2782 (0.0%)	0.96	7/3766 (0.2%)
1	B	0.80	0/2900	1.01	5/3930 (0.1%)
All	All	0.79	1/5682 (0.0%)	0.99	12/7696 (0.2%)

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	B	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	247	GLU	CD-OE2	-8.25	1.16	1.25

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	181	ARG	NE-CZ-NH2	-12.77	113.92	120.30
1	B	370	TYR	CB-CG-CD1	-10.55	114.67	121.00
1	A	370	TYR	CB-CG-CD1	-8.88	115.67	121.00
1	B	66	ARG	NE-CZ-NH1	-7.74	116.43	120.30
1	B	370	TYR	CB-CG-CD2	7.72	125.64	121.00
1	B	181	ARG	NE-CZ-NH1	7.31	123.95	120.30
1	A	268	ARG	NE-CZ-NH2	-6.61	116.99	120.30
1	A	66	ARG	NE-CZ-NH1	-6.53	117.03	120.30
1	A	370	TYR	CB-CG-CD2	6.37	124.82	121.00
1	A	66	ARG	NE-CZ-NH2	5.71	123.16	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	301	ARG	NE-CZ-NH2	-5.55	117.53	120.30
1	A	268	ARG	NE-CZ-NH1	5.00	122.80	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	175	SER	Peptide

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	2717	0	2635	41	1
1	B	2836	0	2761	106	2
2	A	4	0	3	0	0
2	B	4	0	3	0	0
3	A	31	0	19	1	0
3	B	31	0	19	0	0
4	A	4	0	6	0	0
4	B	4	0	6	0	0
5	A	364	0	0	32	4
5	B	364	0	0	69	5
All	All	6359	0	5452	141	9

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 13.

All (141) 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:370:TYR:CE2	5:A:505:HOH:O	1.88	1.25
1:B:332:GLN:NE2	5:B:507:HOH:O	1.77	1.18
1:B:326:LEU:HA	5:B:514:HOH:O	1.51	1.10
1:A:221:LYS:HG3	5:A:503:HOH:O	1.49	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:155:ARG:NH2	5:B:513:HOH:O	1.86	1.07
1:B:331:TRP:HB2	5:B:515:HOH:O	1.51	1.07
1:B:83:HIS:NE2	5:B:512:HOH:O	1.86	1.07
1:B:325:GLY:O	5:B:506:HOH:O	1.77	1.03
1:B:248:ASP:OD1	5:B:508:HOH:O	1.81	0.97
1:A:52[B]:ARG:NH2	5:A:504:HOH:O	1.79	0.97
1:B:111:ALA:N	5:B:515:HOH:O	1.96	0.96
1:B:297:SER:OG	5:B:509:HOH:O	1.84	0.94
1:B:103:THR:OG1	5:B:510:HOH:O	1.84	0.94
1:B:314:ASP:OD2	5:B:511:HOH:O	1.84	0.93
1:B:178:SER:CB	1:B:269:GLN:HE22	1.86	0.87
1:B:251:MET:SD	5:B:811:HOH:O	2.32	0.86
1:B:347:ARG:NH1	1:B:350:GLN:OE1	2.08	0.85
1:B:330:GLY:O	5:B:514:HOH:O	1.95	0.85
1:B:331:TRP:CD1	5:B:519:HOH:O	2.28	0.85
1:B:14:ILE:HG23	5:B:519:HOH:O	1.79	0.82
1:B:332:GLN:O	5:B:516:HOH:O	1.96	0.81
1:B:151:ASP:HB3	5:B:517:HOH:O	1.81	0.80
1:A:367:ASP:OD2	5:A:506:HOH:O	1.99	0.79
1:A:263:SER:OG	5:A:502:HOH:O	2.02	0.77
1:B:333:GLY:N	5:B:502:HOH:O	2.16	0.76
1:B:114:GLU:HB2	5:B:755:HOH:O	1.85	0.76
1:A:69:GLN:NE2	5:A:511:HOH:O	2.18	0.75
1:A:367:ASP:OD2	5:A:508:HOH:O	2.04	0.75
1:B:83:HIS:CD2	5:B:512:HOH:O	2.32	0.73
1:B:199:GLN:O	1:B:203:ARG:HG3	1.89	0.72
1:B:332:GLN:N	5:B:504:HOH:O	2.17	0.72
1:B:178:SER:CB	1:B:269:GLN:NE2	2.52	0.72
1:B:330:GLY:N	5:B:506:HOH:O	2.24	0.71
1:A:370:TYR:HE2	5:A:505:HOH:O	1.41	0.70
1:B:334:ALA:HB2	5:B:514:HOH:O	1.91	0.70
1:B:336:SER:N	5:B:516:HOH:O	2.26	0.68
1:B:373:GLU:OE1	5:B:518:HOH:O	2.11	0.68
1:B:151:ASP:OD2	5:B:517:HOH:O	2.10	0.68
1:A:350:GLN:HG2	5:A:610:HOH:O	1.93	0.68
1:B:334:ALA:N	5:B:514:HOH:O	2.26	0.68
1:B:178:SER:HB2	1:B:269:GLN:NE2	2.09	0.67
1:A:221:LYS:HD3	5:A:507:HOH:O	1.94	0.66
1:B:175:SER:OG	1:B:176:THR:N	2.26	0.66
1:B:331:TRP:CG	5:B:519:HOH:O	2.44	0.66
1:A:364:ASP:OD1	5:A:509:HOH:O	2.13	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:370:TYR:CZ	5:A:505:HOH:O	2.01	0.66
1:A:174:ASP:C	5:A:522:HOH:O	2.34	0.65
1:A:353:GLY:N	5:A:516:HOH:O	2.28	0.65
1:A:364:ASP:CG	5:A:521:HOH:O	2.35	0.65
1:B:39:ASN:HB3	1:B:183:ARG:HG3	1.80	0.64
1:B:334:ALA:C	5:B:505:HOH:O	2.35	0.64
1:B:329:GLY:C	5:B:502:HOH:O	2.36	0.63
1:A:163:SER:HB2	5:A:721:HOH:O	1.99	0.63
1:B:16:TYR:CD2	5:B:507:HOH:O	2.51	0.63
1:A:66:ARG:NH2	5:A:517:HOH:O	2.31	0.62
1:B:289:LYS:NZ	5:B:523:HOH:O	2.32	0.62
1:B:104:LYS:N	5:B:524:HOH:O	2.34	0.61
1:B:111:ALA:HA	5:B:755:HOH:O	2.02	0.60
1:A:364:ASP:CB	5:A:521:HOH:O	2.49	0.59
1:B:183:ARG:HB3	5:B:598:HOH:O	2.03	0.59
1:B:177:VAL:O	1:B:177:VAL:HG12	2.02	0.59
1:B:151:ASP:CB	5:B:517:HOH:O	2.45	0.58
1:A:66:ARG:NH1	5:A:520:HOH:O	2.36	0.58
1:B:14:ILE:HG12	5:B:578:HOH:O	2.03	0.58
1:B:333:GLY:CA	5:B:502:HOH:O	2.52	0.57
1:B:332:GLN:N	5:B:519:HOH:O	2.20	0.57
1:B:162:LYS:HG3	5:B:752:HOH:O	2.05	0.57
1:B:329:GLY:N	5:B:506:HOH:O	2.25	0.57
1:A:289:LYS:CE	1:B:289:LYS:HB3	2.35	0.56
5:A:517:HOH:O	1:B:286:ARG:NH2	2.38	0.56
1:A:69:GLN:HG2	5:A:738:HOH:O	2.06	0.55
1:B:178:SER:HB2	1:B:269:GLN:CD	2.26	0.55
1:A:24:ASP:OD1	5:A:510:HOH:O	2.18	0.54
1:B:195:MET:HB3	1:B:198:VAL:HG22	1.89	0.54
1:B:176:THR:O	1:B:177:VAL:C	2.45	0.54
1:B:110:ARG:C	5:B:515:HOH:O	2.40	0.53
1:B:181:ARG:CG	1:B:181:ARG:O	2.56	0.53
1:B:178:SER:HB2	1:B:269:GLN:OE1	2.09	0.53
1:B:251:MET:HE1	5:B:508:HOH:O	2.07	0.52
1:A:79:GLU:HG3	5:A:532:HOH:O	2.10	0.52
1:B:16:TYR:HD1	5:B:516:HOH:O	1.92	0.52
1:A:289:LYS:HD3	1:B:289:LYS:CD	2.39	0.52
1:B:180:ASN:HA	5:B:817:HOH:O	2.09	0.51
1:B:330:GLY:N	5:B:502:HOH:O	2.43	0.51
1:B:21:ASN:ND2	1:B:24:ASP:H	2.09	0.51
1:B:326:LEU:CA	5:B:514:HOH:O	2.28	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:221:LYS:CD	5:A:507:HOH:O	2.54	0.51
1:B:328:LEU:N	5:B:503:HOH:O	1.93	0.50
1:B:39:ASN:HB3	1:B:183:ARG:CG	2.41	0.50
1:B:101:HIS:HB3	5:B:524:HOH:O	2.11	0.50
1:B:334:ALA:CB	5:B:514:HOH:O	2.56	0.50
1:B:86:LYS:NZ	5:B:537:HOH:O	2.44	0.50
1:B:368:ASN:HD21	1:B:370:TYR:HB2	1.76	0.49
1:A:358:GLU:O	1:B:290:ARG:HD3	2.12	0.49
1:B:16:TYR:N	5:B:507:HOH:O	2.45	0.49
1:A:364:ASP:HB2	5:A:521:HOH:O	2.11	0.49
1:B:21:ASN:HD21	1:B:24:ASP:H	1.60	0.49
1:B:265:HIS:N	5:B:509:HOH:O	2.46	0.48
1:A:290:ARG:HD3	1:B:358:GLU:O	2.14	0.48
1:B:111:ALA:CA	5:B:515:HOH:O	2.50	0.47
1:B:189:PHE:HA	5:B:528:HOH:O	2.15	0.47
1:A:89:PHE:HA	1:A:316:VAL:O	2.15	0.47
1:A:289:LYS:HD3	1:B:289:LYS:HD2	1.97	0.47
1:B:181:ARG:O	1:B:181:ARG:HG3	2.14	0.47
1:B:356:ASN:ND2	1:B:359:ASP:H	2.13	0.46
1:B:325:GLY:C	5:B:503:HOH:O	2.54	0.46
1:B:181:ARG:HG3	1:B:186:LYS:HD2	1.98	0.46
1:B:296:ASP:OD1	5:B:509:HOH:O	2.21	0.46
1:B:329:GLY:N	5:B:542:HOH:O	2.48	0.46
1:A:289:LYS:HE3	5:B:693:HOH:O	2.15	0.45
1:B:330:GLY:C	5:B:504:HOH:O	2.54	0.45
1:B:182:ASP:C	1:B:182:ASP:OD1	2.54	0.45
1:B:182:ASP:O	1:B:183:ARG:HD3	2.17	0.45
1:B:110:ARG:NH1	5:B:543:HOH:O	2.50	0.45
1:A:47:ASP:CG	5:A:504:HOH:O	2.55	0.44
1:B:273:ALA:HB1	1:B:274:PRO:HD2	2.00	0.44
1:B:14:ILE:HG23	5:B:504:HOH:O	2.17	0.44
1:A:176:THR:CG2	5:A:853:HOH:O	2.66	0.44
1:A:244:GLN:HE22	1:A:276:SER:HA	1.84	0.43
1:B:156:ASP:HB3	1:B:201:TYR:CD1	2.53	0.43
1:A:289:LYS:HE2	1:B:289:LYS:HB3	2.01	0.43
1:A:364:ASP:HB2	5:A:517:HOH:O	2.18	0.43
1:B:122:SER:HA	1:B:144:GLN:HE21	1.83	0.43
1:A:241:LYS:HE2	5:A:502:HOH:O	2.18	0.43
1:B:110:ARG:HD2	5:B:768:HOH:O	2.19	0.42
1:A:28:GLU:HG2	5:A:847:HOH:O	2.20	0.42
1:B:89:PHE:HA	1:B:316:VAL:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:144:GLN:NE2	3:A:402:FMN:HN3	2.17	0.42
1:B:183:ARG:NH2	5:B:548:HOH:O	2.51	0.42
1:B:221:LYS:HG3	5:B:531:HOH:O	2.20	0.42
5:A:501:HOH:O	1:B:364:ASP:OD2	2.21	0.41
1:B:177:VAL:O	1:B:177:VAL:CG1	2.68	0.41
1:A:24:ASP:O	1:A:27:GLU:HG2	2.20	0.41
1:B:244:GLN:HE22	1:B:276:SER:HA	1.85	0.41
1:A:182:ASP:C	5:A:589:HOH:O	2.57	0.41
1:B:160:GLU:HB2	1:B:201:TYR:CE2	2.55	0.41
1:B:190:VAL:N	5:B:528:HOH:O	2.37	0.41
1:B:14:ILE:CG2	5:B:519:HOH:O	2.53	0.40
1:B:176:THR:OG1	1:B:220:GLN:OE1	2.27	0.40
1:B:20:VAL:CG2	5:B:757:HOH:O	2.70	0.40
1:B:203:ARG:NH1	5:B:554:HOH:O	2.54	0.40

All (9) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:508:HOH:O	5:B:635:HOH:O[3_655]	1.47	0.73
5:A:801:HOH:O	5:A:801:HOH:O[3_655]	1.97	0.23
5:B:827:HOH:O	5:B:827:HOH:O[3_655]	2.00	0.20
5:B:669:HOH:O	5:B:669:HOH:O[3_655]	2.01	0.19
5:A:524:HOH:O	5:A:787:HOH:O[4_565]	2.02	0.18
1:B:181:ARG:NH2	1:B:301:ARG:NH1[3_655]	2.08	0.12
1:A:68:ALA:N	5:A:503:HOH:O[3_655]	2.13	0.07
5:A:612:HOH:O	5:B:790:HOH:O[7_544]	2.13	0.07
1:B:373:GLU:OE2	5:B:518:HOH:O[3_655]	2.19	0.01

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	345/368 (94%)	336 (97%)	8 (2%)	1 (0%)	41	19
1	B	366/368 (100%)	348 (95%)	9 (2%)	9 (2%)	5	0
All	All	711/736 (97%)	684 (96%)	17 (2%)	10 (1%)	11	1

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	297	SER
1	B	176	THR
1	B	177	VAL
1	B	181	ARG
1	B	297	SER
1	B	180	ASN
1	B	175	SER
1	B	182	ASP
1	B	184	ASP
1	B	178	SER

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	277/292 (95%)	270 (98%)	7 (2%)	47	13
1	B	291/292 (100%)	277 (95%)	14 (5%)	25	2
All	All	568/584 (97%)	547 (96%)	21 (4%)	34	5

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	141	ARG
1	A	175	SER
1	A	176	THR
1	A	198	VAL
1	A	200	ARG
1	A	289	LYS

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Mol	Chain	Res	Type
1	A	342	GLN
1	B	130	GLU
1	B	141	ARG
1	B	143	PHE
1	B	162	LYS
1	B	176	THR
1	B	180	ASN
1	B	186	LYS
1	B	189	PHE
1	B	193	PHE
1	B	195	MET
1	B	203	ARG
1	B	209	MET
1	B	225	ARG
1	B	356	ASN

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	ASN
1	A	39	ASN
1	A	144	GLN
1	A	153	GLN
1	A	244	GLN
1	A	342	GLN
1	B	21	ASN
1	B	83	HIS
1	B	144	GLN
1	B	199	GLN
1	B	244	GLN
1	B	269	GLN
1	B	332	GLN
1	B	355	GLN
1	B	356	ASN
1	B	368	ASN

5.3.3 RNA (i)

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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

6 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	FMN	B	402	-	33,33,33	1.18	5 (15%)	48,50,50	1.02	2 (4%)
4	EDO	B	403	-	3,3,3	0.19	0	2,2,2	0.27	0
2	ACT	B	401	-	3,3,3	1.01	0	3,3,3	0.62	0
4	EDO	A	403	-	3,3,3	0.11	0	2,2,2	0.22	0
2	ACT	A	401	-	3,3,3	1.08	0	3,3,3	0.78	0
3	FMN	A	402	-	33,33,33	1.17	5 (15%)	48,50,50	1.02	3 (6%)

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	FMN	B	402	-	-	1/18/18/18	0/3/3/3
4	EDO	B	403	-	-	1/1/1/1	-
4	EDO	A	403	-	-	0/1/1/1	-
3	FMN	A	402	-	-	2/18/18/18	0/3/3/3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	402	FMN	O3'-C3'	2.75	1.49	1.43
3	B	402	FMN	C2-N1	-2.37	1.31	1.36
3	A	402	FMN	O3'-C3'	2.28	1.48	1.43
3	B	402	FMN	C6-C7	-2.25	1.36	1.39
3	A	402	FMN	P-O3P	-2.20	1.46	1.54
3	A	402	FMN	C6-C7	-2.19	1.36	1.39
3	B	402	FMN	C4A-N5	2.14	1.34	1.30
3	B	402	FMN	P-O3P	-2.09	1.46	1.54
3	A	402	FMN	O4-C4	2.09	1.27	1.23
3	A	402	FMN	P-O2P	-2.06	1.46	1.54

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	402	FMN	C4-N3-C2	-2.52	120.98	125.64
3	B	402	FMN	C4A-C4-N3	2.36	119.19	113.19
3	A	402	FMN	C4A-C4-N3	2.36	119.17	113.19
3	A	402	FMN	C4-C4A-N5	2.34	121.56	118.23
3	A	402	FMN	O4-C4-C4A	-2.01	121.26	126.60

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	402	FMN	C5'-O5'-P-O1P
3	A	402	FMN	C4'-C5'-O5'-P
3	B	402	FMN	C4'-C5'-O5'-P
4	B	403	EDO	O1-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	402	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 B 402

Bond lengths

Bond angles

Torsions

Rings

Ligand FMN A 402
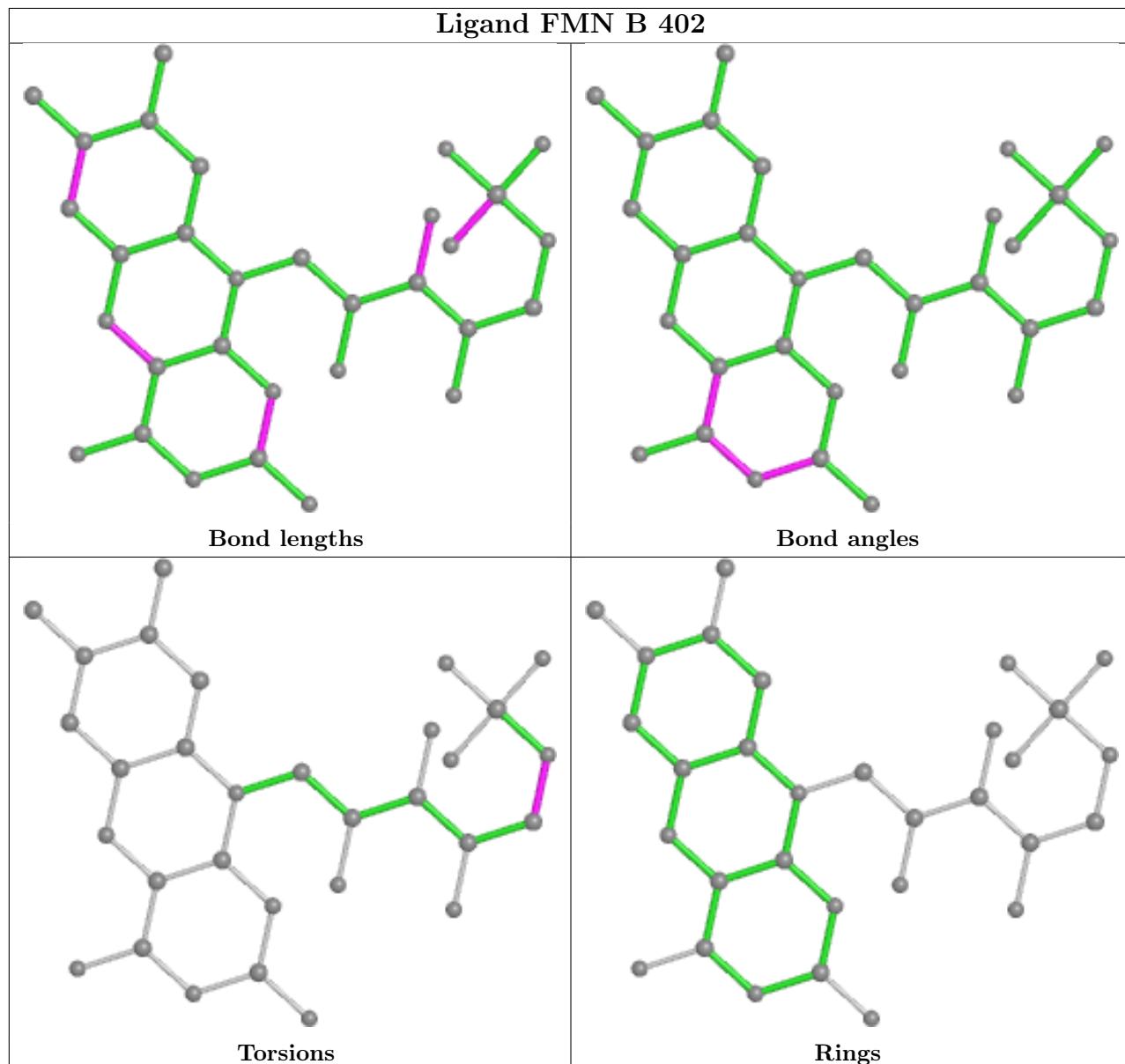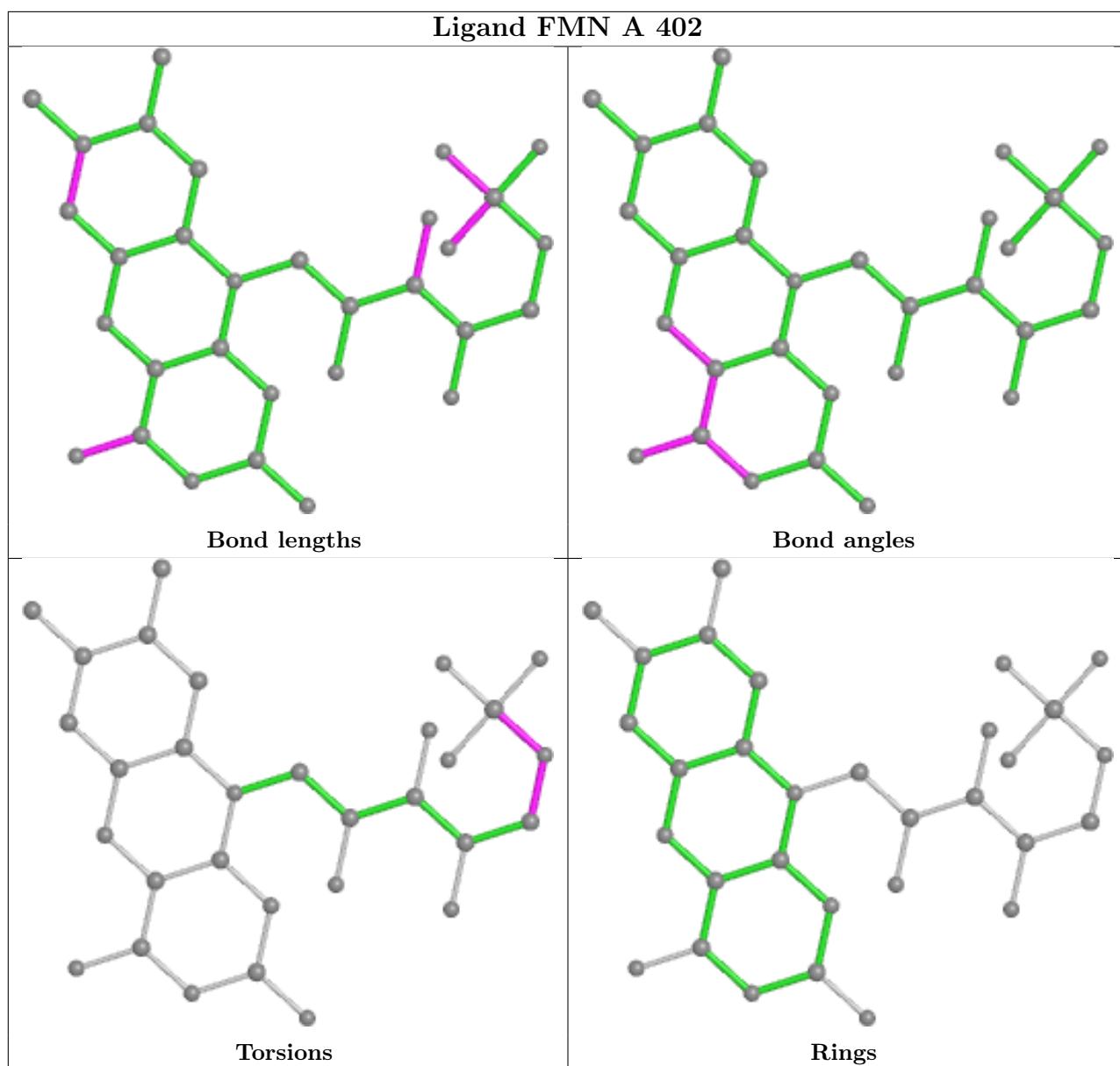
5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	352/368 (95%)	1.14	47 (13%)	3	3	12, 20, 95, 153	0
1	B	368/368 (100%)	0.77	37 (10%)	7	8	13, 21, 49, 131	0
All	All	720/736 (97%)	0.95	84 (11%)	4	4	12, 21, 69, 153	0

All (84) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	208	GLY	25.4
1	A	201	TYR	24.9
1	A	204	GLY	23.1
1	B	178	SER	23.0
1	A	202	LEU	22.9
1	B	183	ARG	20.2
1	A	206	ALA	18.0
1	B	176	THR	17.6
1	B	184	ASP	16.9
1	A	205	THR	15.2
1	A	197	ILE	15.0
1	B	177	VAL	14.4
1	B	185	VAL	13.5
1	A	209	MET	12.9
1	A	203	ARG	12.9
1	A	191	TYR	11.1
1	A	200	ARG	11.0
1	A	198	VAL	9.4
1	A	193	PHE	8.9
1	B	190	VAL	8.1
1	A	215	TYR	7.9
1	A	199	GLN	7.2
1	A	207	GLU	7.2
1	B	179	GLY	6.9

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Mol	Chain	Res	Type	RSRZ
1	B	201	TYR	6.7
1	B	191	TYR	6.3
1	A	176	THR	6.2
1	B	214	ILE	6.1
1	B	180	ASN	6.1
1	A	194	GLY	6.0
1	B	211	LEU	6.0
1	A	196	PRO	6.0
1	B	187	ASN	5.8
1	B	188	LYS	5.4
1	B	206	ALA	5.4
1	A	157	ILE	5.3
1	B	189	PHE	5.3
1	A	192	PRO	4.9
1	B	215	TYR	4.9
1	A	129	PHE	4.8
1	B	182	ASP	4.7
1	A	124	TYR	4.5
1	A	143	PHE	4.5
1	A	7	GLU	4.5
1	A	195	MET	4.3
1	B	186	LYS	4.2
1	B	7	GLU	4.2
1	A	181	ARG	4.0
1	B	209	MET	3.7
1	B	203	ARG	3.7
1	A	155	ARG	3.7
1	B	193	PHE	3.7
1	B	175	SER	3.7
1	B	200	ARG	3.6
1	B	210	SER	3.4
1	A	130	GLU	3.3
1	A	180	ASN	3.3
1	A	128	THR	2.9
1	B	194	GLY	2.9
1	A	160	GLU	2.8
1	B	71	VAL	2.8
1	A	182	ASP	2.8
1	B	212	ASN	2.7
1	A	163	SER	2.6
1	B	197	ILE	2.6
1	B	195	MET	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	151	ASP	2.6
1	B	143	PHE	2.6
1	B	134	GLU	2.5
1	A	134	GLU	2.5
1	A	153	GLN	2.3
1	A	216	GLY	2.3
1	A	159	ASP	2.2
1	A	137	ASN	2.2
1	B	213	ASN	2.2
1	B	129	PHE	2.2
1	A	71	VAL	2.2
1	A	294	VAL	2.2
1	A	175	SER	2.1
1	A	260	ILE	2.1
1	A	217	ALA	2.1
1	A	225	ARG	2.1
1	A	152	GLN	2.0
1	B	207	GLU	2.0

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	ACT	A	401	4/4	0.77	0.16	36,37,40,44	0
2	ACT	B	401	4/4	0.85	0.12	30,32,33,36	0
4	EDO	A	403	4/4	0.88	0.12	39,42,44,53	0
4	EDO	B	403	4/4	0.89	0.12	35,36,37,47	0
3	FMN	B	402	31/31	0.97	0.07	13,16,21,22	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
3	FMN	A	402	31/31	0.98	0.08	13,16,20,23	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around FMN B 402:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

Electron density around FMN A 402:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

6.5 Other polymers ⓘ

There are no such residues in this entry.