



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 16, 2025 – 06:11 PM EDT

PDB ID : 9CB8 / pdb_00009cb8
Title : Crystal structure of dihydroorotate dehydrogenase from Leishmania brasiliensis in complex with 5-benzylidenepyrimidine-2,4,6(1H,3H,5H)-trione
Authors : Froes, T.Q.; Vaidergorn, M.M.; dos Santos, T.; Leite, P.I.P.L.; Godoi, B.F.; Emery, F.S.; Nonato, M.C.
Deposited on : 2024-06-18
Resolution : 1.75 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 Phenix2.0rc1
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.44

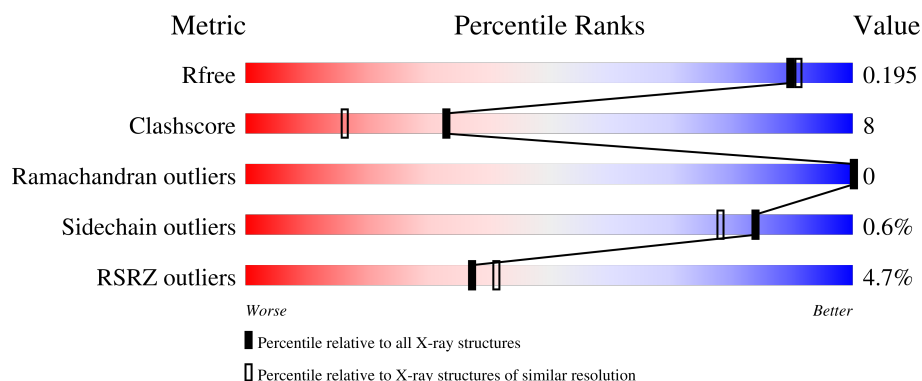
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.75 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))
R_{free}	164625	2888 (1.76-1.76)
Clashscore	180529	3097 (1.76-1.76)
Ramachandran outliers	177936	3072 (1.76-1.76)
Sidechain outliers	177891	3072 (1.76-1.76)
RSRZ outliers	164620	2887 (1.76-1.76)

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 $\leq 5\%$. 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	347	
1	B	347	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	GOL	B	401	-	-	X	-
3	GOL	B	403	-	-	X	-
4	A1AVS	B	404	-	X	-	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9650 atoms, of which 4622 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 Dihydroorotate dehydrogenase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	304	Total	C	H	N	O	S	0	2	0
			4450	1455	2189	372	416	18			
1	B	313	Total	C	H	N	O	S	0	8	0
			4732	1529	2345	400	439	19			

There are 68 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-33	MET	-	initiating methionine	UNP E9AI53
A	-32	GLY	-	expression tag	UNP E9AI53
A	-31	SER	-	expression tag	UNP E9AI53
A	-30	SER	-	expression tag	UNP E9AI53
A	-29	HIS	-	expression tag	UNP E9AI53
A	-28	HIS	-	expression tag	UNP E9AI53
A	-27	HIS	-	expression tag	UNP E9AI53
A	-26	HIS	-	expression tag	UNP E9AI53
A	-25	HIS	-	expression tag	UNP E9AI53
A	-24	HIS	-	expression tag	UNP E9AI53
A	-23	SER	-	expression tag	UNP E9AI53
A	-22	SER	-	expression tag	UNP E9AI53
A	-21	GLY	-	expression tag	UNP E9AI53
A	-20	LEU	-	expression tag	UNP E9AI53
A	-19	VAL	-	expression tag	UNP E9AI53
A	-18	PRO	-	expression tag	UNP E9AI53
A	-17	ARG	-	expression tag	UNP E9AI53
A	-16	GLY	-	expression tag	UNP E9AI53
A	-15	SER	-	expression tag	UNP E9AI53
A	-14	HIS	-	expression tag	UNP E9AI53
A	-13	MET	-	expression tag	UNP E9AI53
A	-12	ALA	-	expression tag	UNP E9AI53
A	-11	SER	-	expression tag	UNP E9AI53
A	-10	MET	-	expression tag	UNP E9AI53
A	-9	THR	-	expression tag	UNP E9AI53

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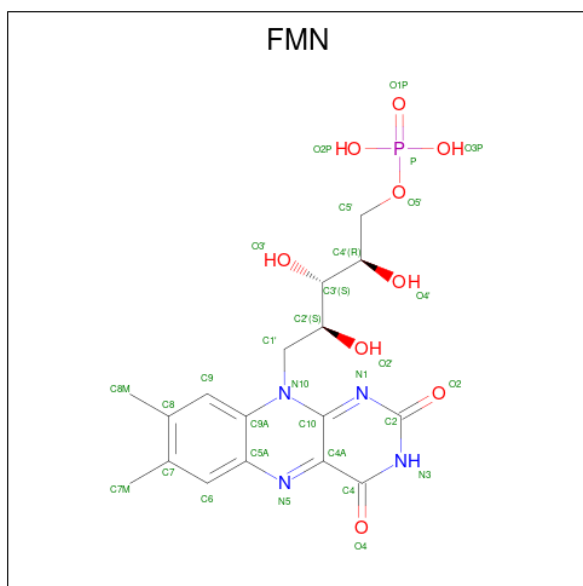
Chain	Residue	Modelled	Actual	Comment	Reference
A	-8	GLY	-	expression tag	UNP E9AI53
A	-7	GLY	-	expression tag	UNP E9AI53
A	-6	GLY	-	expression tag	UNP E9AI53
A	-5	GLN	-	expression tag	UNP E9AI53
A	-4	MET	-	expression tag	UNP E9AI53
A	-3	GLY	-	expression tag	UNP E9AI53
A	-2	ARG	-	expression tag	UNP E9AI53
A	-1	GLY	-	expression tag	UNP E9AI53
A	0	SER	-	expression tag	UNP E9AI53
B	-33	MET	-	initiating methionine	UNP E9AI53
B	-32	GLY	-	expression tag	UNP E9AI53
B	-31	SER	-	expression tag	UNP E9AI53
B	-30	SER	-	expression tag	UNP E9AI53
B	-29	HIS	-	expression tag	UNP E9AI53
B	-28	HIS	-	expression tag	UNP E9AI53
B	-27	HIS	-	expression tag	UNP E9AI53
B	-26	HIS	-	expression tag	UNP E9AI53
B	-25	HIS	-	expression tag	UNP E9AI53
B	-24	HIS	-	expression tag	UNP E9AI53
B	-23	SER	-	expression tag	UNP E9AI53
B	-22	SER	-	expression tag	UNP E9AI53
B	-21	GLY	-	expression tag	UNP E9AI53
B	-20	LEU	-	expression tag	UNP E9AI53
B	-19	VAL	-	expression tag	UNP E9AI53
B	-18	PRO	-	expression tag	UNP E9AI53
B	-17	ARG	-	expression tag	UNP E9AI53
B	-16	GLY	-	expression tag	UNP E9AI53
B	-15	SER	-	expression tag	UNP E9AI53
B	-14	HIS	-	expression tag	UNP E9AI53
B	-13	MET	-	expression tag	UNP E9AI53
B	-12	ALA	-	expression tag	UNP E9AI53
B	-11	SER	-	expression tag	UNP E9AI53
B	-10	MET	-	expression tag	UNP E9AI53
B	-9	THR	-	expression tag	UNP E9AI53
B	-8	GLY	-	expression tag	UNP E9AI53
B	-7	GLY	-	expression tag	UNP E9AI53
B	-6	GLY	-	expression tag	UNP E9AI53
B	-5	GLN	-	expression tag	UNP E9AI53
B	-4	MET	-	expression tag	UNP E9AI53
B	-3	GLY	-	expression tag	UNP E9AI53
B	-2	ARG	-	expression tag	UNP E9AI53
B	-1	GLY	-	expression tag	UNP E9AI53

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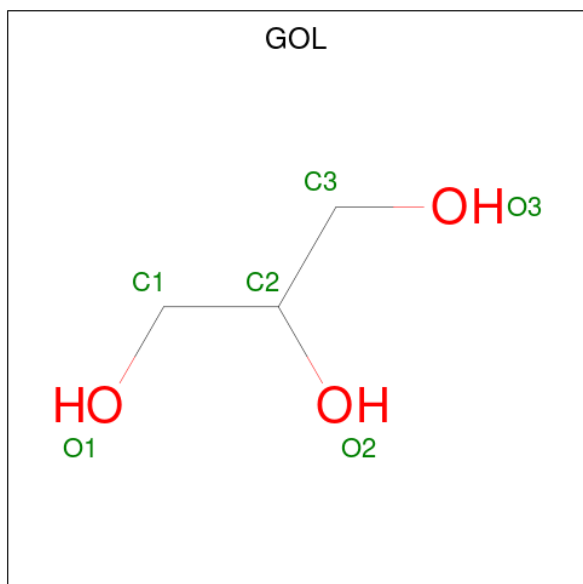
Chain	Residue	Modelled	Actual	Comment	Reference
B	0	SER	-	expression tag	UNP E9AI53

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



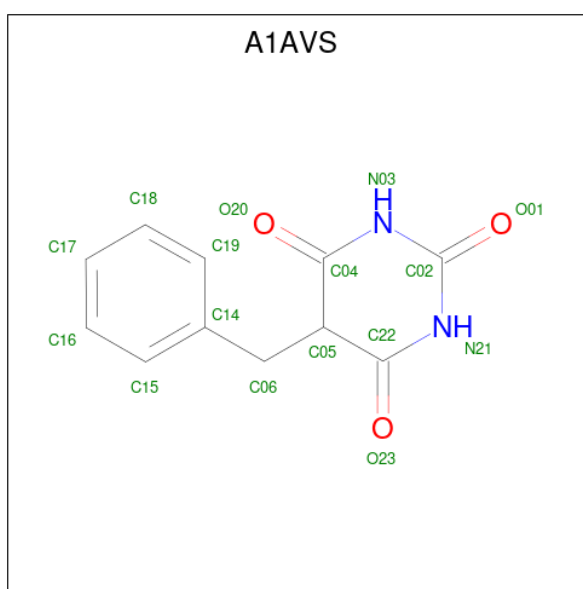
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
2	A	1	Total	C	H	N	O	P	0	0
			50	17	19	4	9	1		
2	B	1	Total	C	H	N	O	P	0	0
			50	17	19	4	9	1		

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C H O 14 3 8 3	0	0
3	A	1	Total C H O 14 3 8 3	0	0
3	B	1	Total C H O 14 3 8 3	0	0
3	B	1	Total C H O 14 3 8 3	0	0

- Molecule 4 is 5-benzyl-1,3-diazinane-2,4,6-trione (CCD ID: A1AVS) (formula: $C_{11}H_{10}N_2O_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C H N O 25 11 9 2 3	0	0
4	B	1	Total C H N O 25 11 9 2 3	0	0

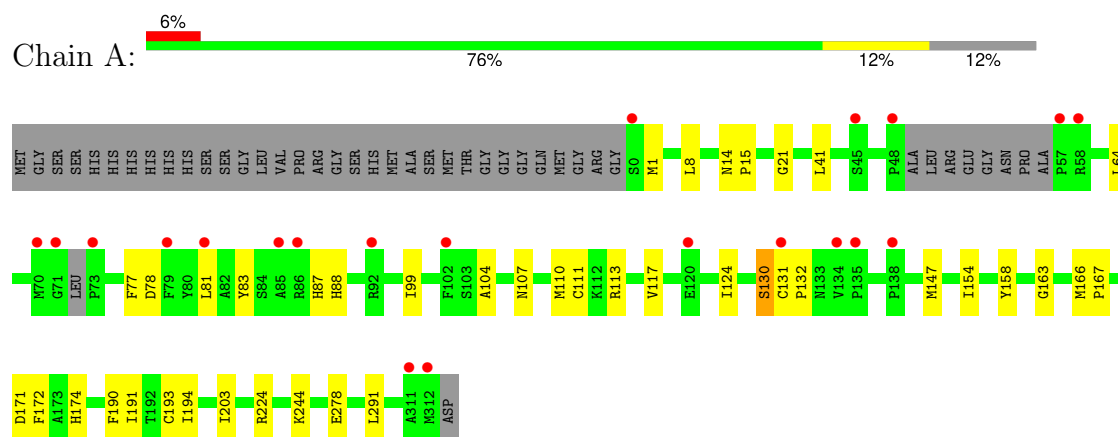
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	83	Total O 83 83	0	0
5	B	179	Total O 179 179	0	0

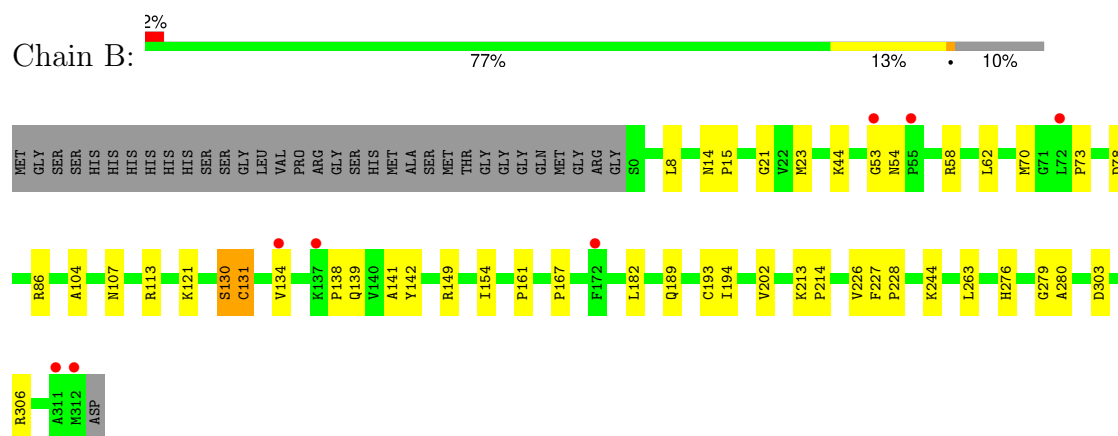
3 Residue-property plots [i](#)

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 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: Dihydroorotate dehydrogenase



- Molecule 1: Dihydroorotate dehydrogenase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	61.54Å 104.78Å 106.84Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.89 – 1.75 39.89 – 1.75	Depositor EDS
% Data completeness (in resolution range)	99.0 (39.89-1.75) 98.9 (39.89-1.75)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.39 (at 1.75Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.169 , 0.194 0.170 , 0.195	Depositor DCC
R_{free} test set	4244 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	36.0	Xtriage
Anisotropy	0.237	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.43 , 41.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.004 for -h,l,k	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	9650	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.29% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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: A1AVS, FMN, GOL

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	0.52	3/2321 (0.1%)	0.53	0/3143
1	B	0.53	3/2477 (0.1%)	0.57	0/3355
All	All	0.53	6/4798 (0.1%)	0.55	0/6498

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	131	CYS	CA-C	-16.56	1.34	1.53
1	B	131	CYS	CA-C	-14.96	1.36	1.53
1	A	130	SER	C-N	5.76	1.42	1.33
1	B	130	SER	C-N	5.70	1.42	1.33
1	A	131	CYS	C-O	-5.34	1.17	1.24
1	B	131	CYS	C-O	-5.07	1.18	1.24

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	2261	2189	2179	30	0
1	B	2387	2345	2309	42	1
2	A	31	19	19	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	31	19	19	1	0
3	A	12	16	16	3	0
3	B	12	16	16	14	0
4	A	16	9	0	0	0
4	B	16	9	0	0	0
5	A	83	0	0	1	1
5	B	179	0	0	6	2
All	All	5028	4622	4558	72	2

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 (72) 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:B:86:ARG:NH1	5:B:501:HOH:O	1.84	1.09
1:B:139[B]:GLN:HG3	1:B:142:TYR:CD2	2.05	0.92
1:A:78:ASP:OD1	1:A:113:ARG:NH2	2.10	0.85
1:B:23[A]:MET:HE3	5:B:597:HOH:O	1.80	0.82
1:A:107:ASN:HB3	1:A:154:ILE:HD11	1.66	0.76
1:B:104:ALA:H	3:B:403:GOL:H32	1.50	0.76
1:B:121:LYS:NZ	5:B:503:HOH:O	2.17	0.76
1:B:149:ARG:HH12	3:B:403:GOL:H31	1.56	0.71
1:B:104:ALA:H	3:B:403:GOL:C3	2.05	0.69
1:A:174:HIS:NE2	3:A:403:GOL:H11	2.11	0.65
1:B:303:ASP:OD1	1:B:306:ARG:NH1	2.29	0.65
1:B:161:PRO:HB2	1:B:189[B]:GLN:CD	2.25	0.62
1:B:149:ARG:HH12	3:B:403:GOL:C3	2.14	0.61
1:A:172:PHE:HB2	3:B:401:GOL:H12	1.84	0.59
1:B:14:ASN:HB2	1:B:15:PRO:HD2	1.83	0.59
1:B:23[A]:MET:CE	5:B:597:HOH:O	2.42	0.57
1:B:58:ARG:HG3	1:B:70:MET:SD	2.44	0.57
1:B:138:PRO:HG3	3:B:401:GOL:H11	1.86	0.57
1:B:78:ASP:OD1	1:B:113:ARG:NH2	2.31	0.56
1:A:172:PHE:H	3:B:401:GOL:C3	2.18	0.56
1:A:171:ASP:HB2	3:B:401:GOL:H2	1.87	0.55
3:B:401:GOL:O1	5:B:502:HOH:O	2.10	0.53
1:B:139[B]:GLN:HG3	1:B:142:TYR:CE2	2.43	0.53
1:B:161:PRO:HB2	1:B:189[B]:GLN:OE1	2.08	0.53
1:B:21:GLY:HA3	2:B:402:FMN:N5	2.23	0.53
1:A:21:GLY:HA3	2:A:401:FMN:N5	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:23[B]:MET:HE1	1:B:280:ALA:HB2	1.91	0.52
1:A:172:PHE:HB2	3:B:401:GOL:H32	1.92	0.52
1:B:107:ASN:HB3	1:B:154:ILE:HD11	1.92	0.50
1:B:23[A]:MET:O	1:B:23[A]:MET:HG2	2.11	0.50
1:A:104:ALA:H	3:A:402:GOL:HO2	1.59	0.48
1:B:149:ARG:HH22	3:B:403:GOL:H12	1.78	0.48
1:A:191:ILE:HD11	1:A:244:LYS:HD2	1.95	0.48
1:B:138:PRO:HA	3:B:401:GOL:O2	2.14	0.47
1:A:163:GLY:HA3	1:A:190:PHE:CZ	2.50	0.47
1:B:70:MET:HB2	5:B:520:HOH:O	2.14	0.47
1:B:8:LEU:HD22	1:B:189[B]:GLN:CD	2.40	0.47
1:B:53:GLY:HA3	1:B:73:PRO:HB3	1.97	0.46
1:B:62:LEU:HD21	1:B:202:VAL:HG21	1.96	0.46
1:A:14:ASN:HB2	1:A:15:PRO:HD2	1.98	0.46
1:B:23[B]:MET:O	1:B:23[B]:MET:HG2	2.16	0.46
1:B:23[A]:MET:HE1	1:B:279:GLY:HA2	1.98	0.45
1:A:1:MET:HE3	1:A:291:LEU:HD22	1.97	0.45
1:B:149:ARG:NH1	3:B:403:GOL:H31	2.28	0.45
1:A:111:CYS:HB3	1:A:158:TYR:CD1	2.51	0.45
1:B:54:ASN:HB3	1:B:214:PRO:HG3	1.99	0.45
1:A:64:LEU:O	1:A:224:ARG:HB2	2.17	0.44
1:A:203:ILE:HG21	1:B:263:LEU:HD23	1.99	0.44
1:A:1:MET:HE3	1:A:1:MET:HB2	1.72	0.44
1:A:193:CYS:HA	1:A:194:ILE:HA	1.83	0.44
1:A:83:TYR:CE2	1:A:88:HIS:HB2	2.53	0.44
1:B:227:PHE:HB3	1:B:228:PRO:HD3	1.99	0.44
1:B:139[B]:GLN:H	1:B:139[B]:GLN:HG2	1.35	0.43
1:B:182:LEU:O	1:B:244:LYS:HE3	2.19	0.43
1:A:41:LEU:HD23	1:A:41:LEU:N	2.34	0.43
1:A:83:TYR:HA	1:A:87:HIS:HB2	2.00	0.43
1:B:44:LYS:HE2	1:B:73:PRO:O	2.19	0.43
1:B:104:ALA:N	3:B:403:GOL:H32	2.27	0.42
1:A:8:LEU:HD13	1:A:124:ILE:HD13	2.00	0.42
1:A:99:ILE:O	1:A:99:ILE:HG13	2.19	0.42
1:B:131:CYS:HB3	1:B:134:VAL:HG23	2.01	0.42
1:A:77:PHE:CG	1:A:110:MET:HG2	2.54	0.42
1:B:54:ASN:HB3	1:B:214:PRO:CG	2.50	0.42
1:B:141:ALA:HB3	1:B:167:PRO:CD	2.50	0.42
1:A:130:SER:HB3	1:A:167:PRO:HD3	2.02	0.41
1:A:174:HIS:NE2	3:A:403:GOL:C1	2.82	0.41
1:B:193:CYS:HA	1:B:194:ILE:HA	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:81:LEU:HD11	1:A:117:VAL:HG21	2.03	0.41
1:B:213:LYS:HB3	1:B:214:PRO:HD3	2.03	0.41
1:A:147:MET:HE1	1:A:166:MET:HE1	2.03	0.40
1:A:278:GLU:OE2	5:A:501:HOH:O	2.22	0.40
1:A:130:SER:HB3	1:A:167:PRO:CD	2.51	0.40

All (2) 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:A:564:HOH:O	5:B:551:HOH:O[3_544]	2.16	0.04
1:B:276:HIS:ND1	5:B:501:HOH:O[4_454]	2.16	0.04

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	300/347 (86%)	290 (97%)	10 (3%)	0	100	100
1	B	319/347 (92%)	304 (95%)	15 (5%)	0	100	100
All	All	619/694 (89%)	594 (96%)	25 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	229/273 (84%)	228 (100%)	1 (0%)	89	86
1	B	249/273 (91%)	247 (99%)	2 (1%)	79	71
All	All	478/546 (88%)	475 (99%)	3 (1%)	84	78

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	132	PRO
1	B	130	SER
1	B	226	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	199	ASN

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](#)

8 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	GOL	A	402	-	5,5,5	0.29	0	5,5,5	0.25	0
3	GOL	B	403	-	5,5,5	0.27	0	5,5,5	0.53	0
4	A1AVS	A	404	1	17,17,17	4.14	13 (76%)	20,23,23	2.84	8 (40%)
3	GOL	B	401	-	5,5,5	0.23	0	5,5,5	0.38	0
2	FMN	A	401	-	33,33,33	1.07	2 (6%)	48,50,50	1.15	7 (14%)
2	FMN	B	402	-	33,33,33	1.13	2 (6%)	48,50,50	1.24	6 (12%)
3	GOL	A	403	-	5,5,5	0.31	0	5,5,5	0.46	0
4	A1AVS	B	404	1	17,17,17	4.24	13 (76%)	20,23,23	2.92	8 (40%)

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	GOL	A	402	-	-	0/4/4/4	-
3	GOL	B	403	-	-	0/4/4/4	-
4	A1AVS	A	404	1	-	2/4/20/20	0/2/2/2
3	GOL	B	401	-	-	2/4/4/4	-
2	FMN	A	401	-	-	2/18/18/18	0/3/3/3
2	FMN	B	402	-	-	2/18/18/18	0/3/3/3
3	GOL	A	403	-	-	4/4/4/4	-
4	A1AVS	B	404	1	-	4/4/20/20	0/2/2/2

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	404	A1AVS	C16-C15	8.48	1.53	1.38
4	B	404	A1AVS	C16-C15	8.43	1.53	1.38
4	B	404	A1AVS	C19-C14	8.04	1.54	1.38
4	A	404	A1AVS	C19-C14	7.42	1.53	1.38
4	A	404	A1AVS	C18-C17	6.71	1.53	1.38
4	B	404	A1AVS	C18-C17	6.70	1.53	1.38
4	B	404	A1AVS	C22-N21	5.23	1.46	1.37
4	A	404	A1AVS	C04-N03	4.96	1.46	1.37
4	B	404	A1AVS	O20-C04	-4.66	1.14	1.23
4	A	404	A1AVS	O23-C22	-4.65	1.14	1.23
2	A	401	FMN	C4A-N5	3.86	1.39	1.30
2	B	402	FMN	C4A-N5	3.70	1.38	1.30
4	B	404	A1AVS	C18-C19	-3.64	1.32	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	404	A1AVS	C18-C19	-3.60	1.32	1.38
4	A	404	A1AVS	C22-N21	3.45	1.43	1.37
4	B	404	A1AVS	C04-N03	3.35	1.43	1.37
4	A	404	A1AVS	O20-C04	-3.18	1.17	1.23
4	A	404	A1AVS	C15-C14	-3.18	1.32	1.38
2	A	401	FMN	C10-N1	3.08	1.39	1.33
4	B	404	A1AVS	C15-C14	-2.94	1.33	1.38
4	B	404	A1AVS	C17-C16	-2.86	1.31	1.38
4	B	404	A1AVS	C05-C22	2.77	1.54	1.52
4	A	404	A1AVS	C17-C16	-2.75	1.32	1.38
2	B	402	FMN	C10-N1	2.70	1.38	1.33
4	B	404	A1AVS	O01-C02	-2.67	1.17	1.23
4	B	404	A1AVS	C02-N21	2.65	1.41	1.37
4	B	404	A1AVS	O23-C22	-2.58	1.18	1.23
4	A	404	A1AVS	O01-C02	-2.53	1.18	1.23
4	A	404	A1AVS	C02-N03	2.49	1.41	1.37
4	A	404	A1AVS	C05-C04	2.16	1.54	1.52

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	404	A1AVS	C05-C04-N03	8.21	125.86	116.20
4	A	404	A1AVS	C05-C22-N21	8.09	125.72	116.20
4	A	404	A1AVS	C05-C04-N03	4.91	121.97	116.20
4	B	404	A1AVS	C04-N03-C02	-4.50	120.58	126.23
4	A	404	A1AVS	C22-N21-C02	-4.38	120.73	126.23
4	B	404	A1AVS	C05-C22-N21	4.31	121.28	116.20
4	B	404	A1AVS	O20-C04-N03	-4.04	113.91	121.10
4	A	404	A1AVS	O23-C22-N21	-3.47	114.93	121.10
4	B	404	A1AVS	C14-C06-C05	3.40	120.42	113.31
2	B	402	FMN	C4-N3-C2	-3.20	119.96	125.64
4	A	404	A1AVS	C04-N03-C02	-3.06	122.38	126.23
4	B	404	A1AVS	O01-C02-N03	-3.05	116.44	121.86
4	B	404	A1AVS	C22-N21-C02	-2.87	122.62	126.23
2	B	402	FMN	C4A-C10-N10	2.76	120.44	116.48
4	B	404	A1AVS	N21-C02-N03	2.72	120.02	115.74
2	B	402	FMN	O4-C4-C4A	-2.64	119.57	126.53
2	B	402	FMN	C4A-C4-N3	2.59	119.85	113.25
4	A	404	A1AVS	N21-C02-N03	2.59	119.81	115.74
2	A	401	FMN	C4-N3-C2	-2.56	121.10	125.64
4	A	404	A1AVS	O01-C02-N21	-2.52	117.38	121.86
2	A	401	FMN	C4A-C4-N3	2.52	119.66	113.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	402	FMN	C5A-C9A-N10	2.42	120.15	117.97
2	A	401	FMN	C5A-C9A-N10	2.37	120.11	117.97
2	A	401	FMN	C4A-C10-N10	2.31	119.79	116.48
4	A	404	A1AVS	C06-C14-C19	-2.30	116.63	120.90
2	B	402	FMN	C9-C9A-N10	-2.21	118.88	121.85
2	A	401	FMN	C9A-C5A-N5	-2.16	120.16	122.45
2	A	401	FMN	O4-C4-C4A	-2.13	120.90	126.53
2	A	401	FMN	C10-C4A-N5	-2.10	120.53	124.81

There are no chirality outliers.

All (16) torsion outliers are listed below:

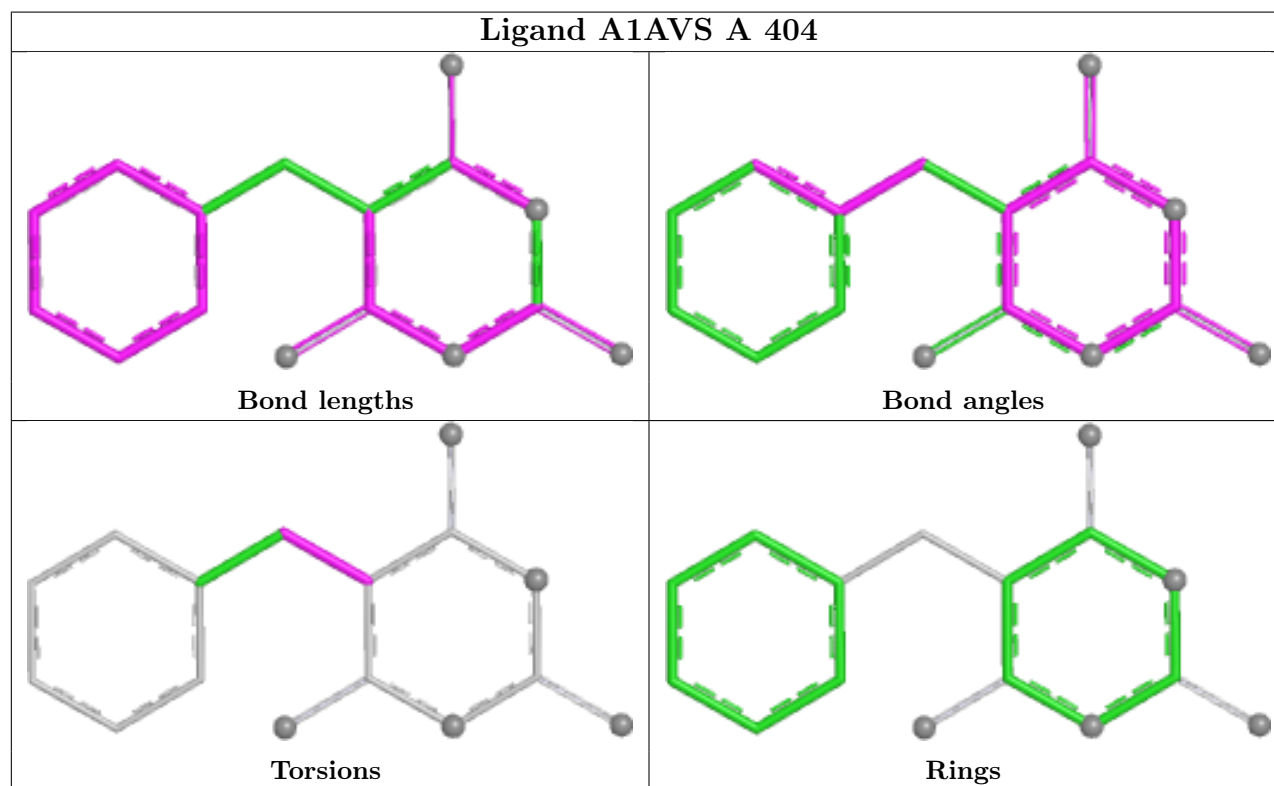
Mol	Chain	Res	Type	Atoms
4	A	404	A1AVS	C04-C05-C06-C14
4	A	404	A1AVS	C22-C05-C06-C14
4	B	404	A1AVS	C22-C05-C06-C14
4	B	404	A1AVS	C05-C06-C14-C15
4	B	404	A1AVS	C05-C06-C14-C19
3	A	403	GOL	O1-C1-C2-O2
3	A	403	GOL	O2-C2-C3-O3
3	A	403	GOL	O1-C1-C2-C3
3	A	403	GOL	C1-C2-C3-O3
3	B	401	GOL	C1-C2-C3-O3
3	B	401	GOL	O2-C2-C3-O3
2	B	402	FMN	C4'-C5'-O5'-P
2	A	401	FMN	C4'-C5'-O5'-P
2	A	401	FMN	C2'-C3'-C4'-O4'
2	B	402	FMN	C2'-C3'-C4'-O4'
4	B	404	A1AVS	C04-C05-C06-C14

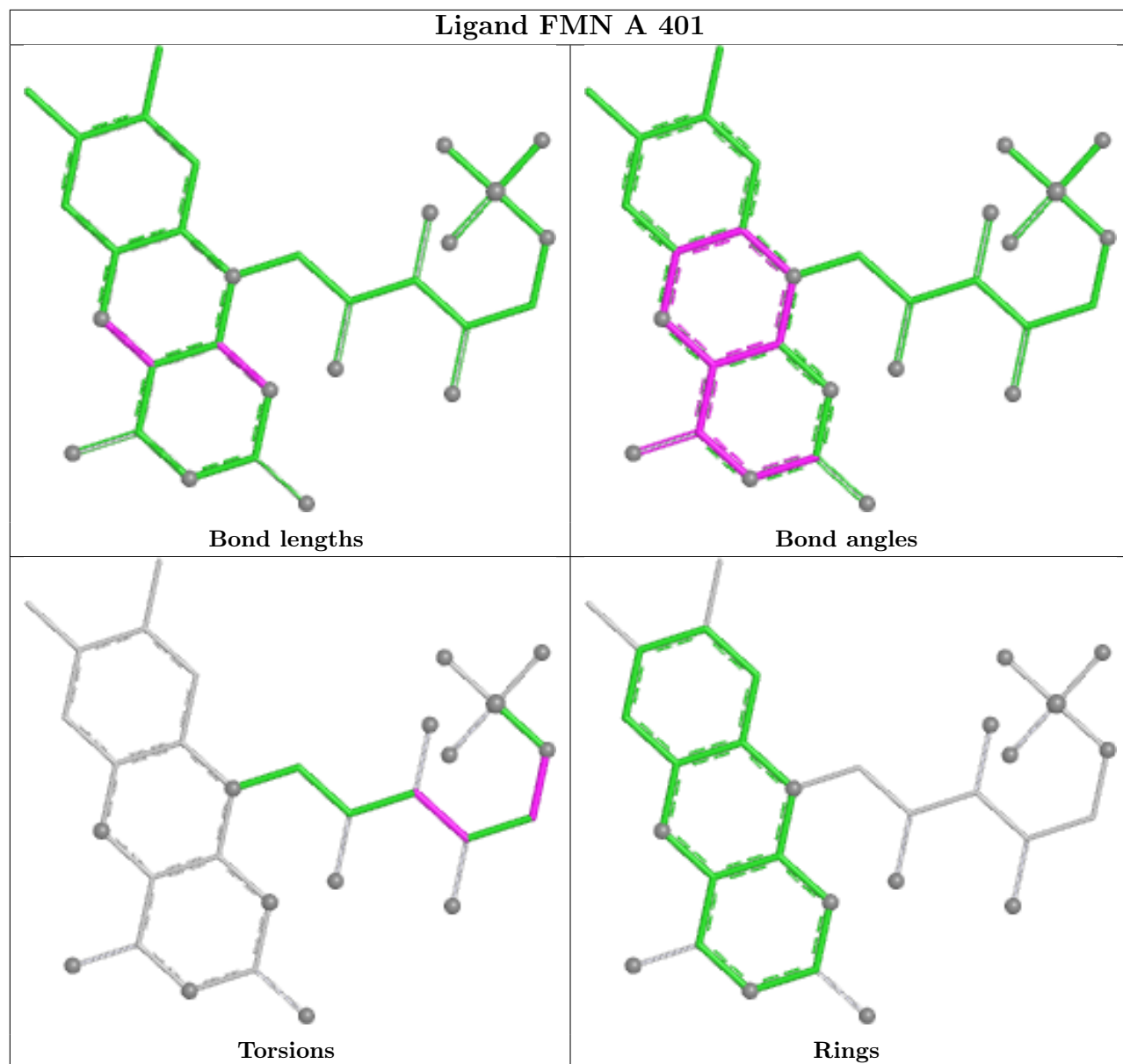
There are no ring outliers.

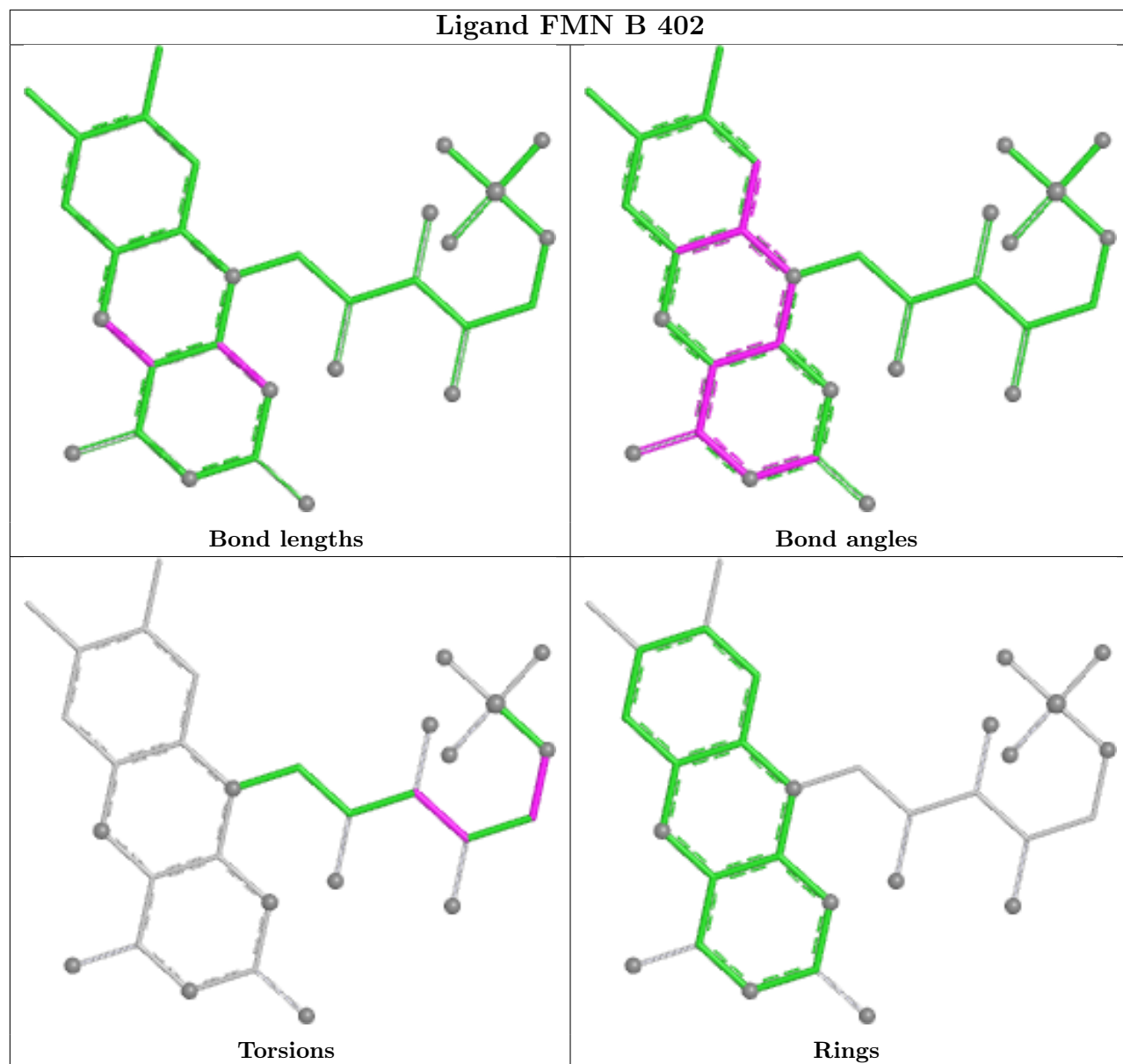
6 monomers are involved in 19 short contacts:

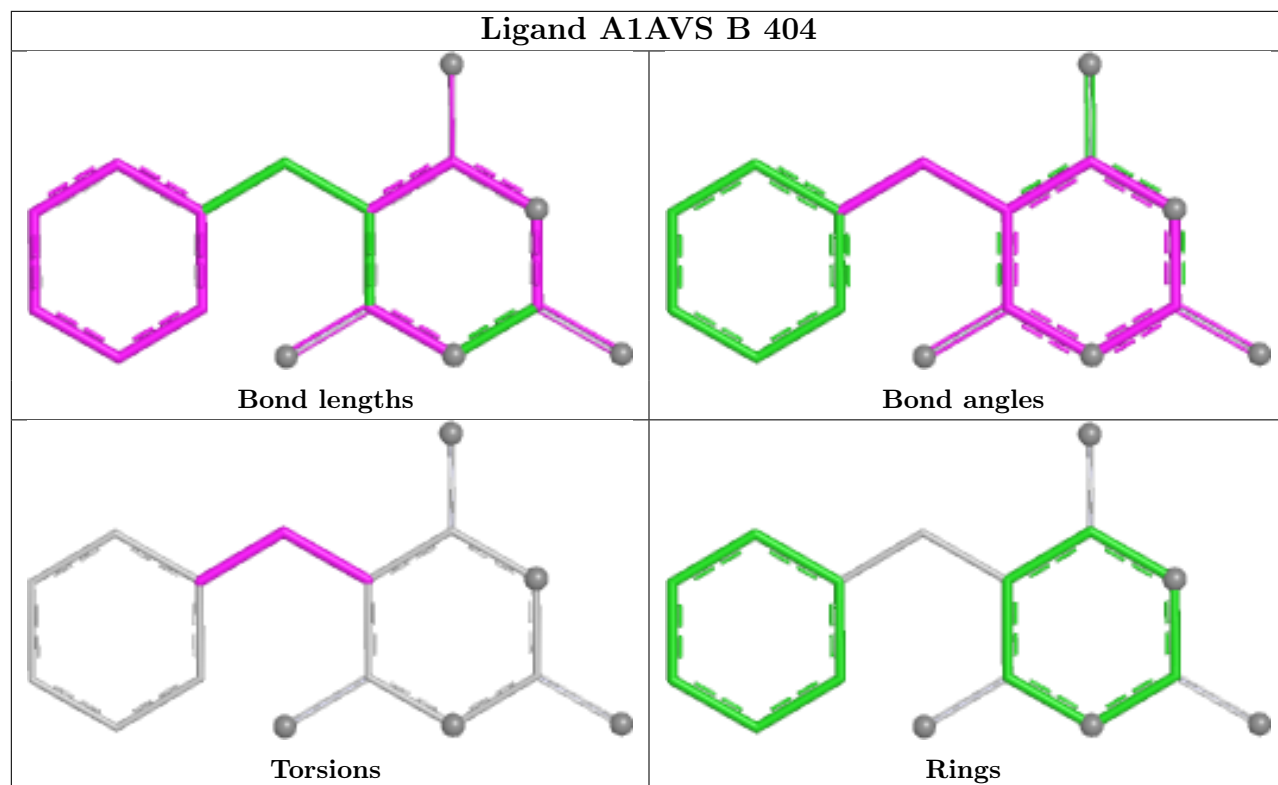
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	402	GOL	1	0
3	B	403	GOL	7	0
3	B	401	GOL	7	0
2	A	401	FMN	1	0
2	B	402	FMN	1	0
3	A	403	GOL	2	0

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

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	304/347 (87%)	0.40	21 (6%) 24 27	18, 45, 80, 93	6 (1%)
1	B	313/347 (90%)	-0.10	8 (2%) 57 64	16, 35, 60, 83	6 (1%)
All	All	617/694 (88%)	0.15	29 (4%) 37 41	16, 39, 76, 93	12 (1%)

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	73	PRO	6.1
1	B	311	ALA	3.6
1	A	102	PHE	3.2
1	B	53	GLY	3.2
1	A	135	PRO	3.0
1	A	48	PRO	2.9
1	B	72	LEU	2.8
1	A	70	MET	2.8
1	B	312	MET	2.7
1	A	131	CYS	2.7
1	B	134	VAL	2.7
1	A	71	GLY	2.7
1	A	120	GLU	2.7
1	A	92	ARG	2.7
1	A	85	ALA	2.6
1	A	58	ARG	2.5
1	A	311	ALA	2.5
1	A	134	VAL	2.5
1	A	0	SER	2.4
1	A	138	PRO	2.3
1	A	81	LEU	2.3
1	A	86	ARG	2.3
1	B	137	LYS	2.3
1	A	79	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	312	MET	2.1
1	B	55	PRO	2.1
1	A	57	PRO	2.1
1	B	172	PHE	2.0
1	A	45	SER	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

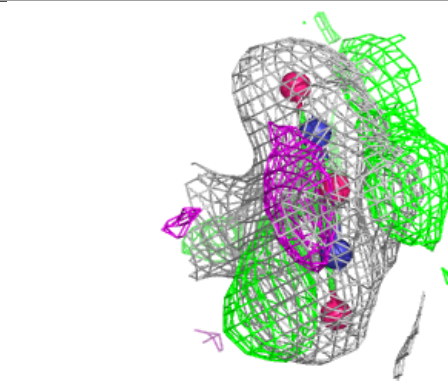
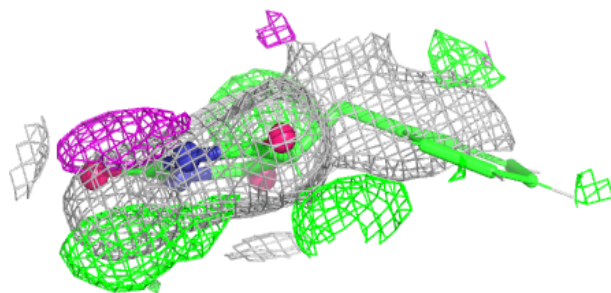
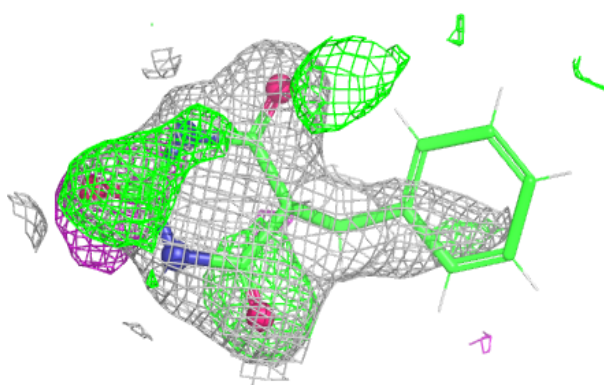
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	GOL	B	403	6/6	0.74	0.15	55,69,83,88	0
3	GOL	A	403	6/6	0.76	0.14	68,81,95,96	0
3	GOL	A	402	6/6	0.76	0.14	76,92,103,103	0
3	GOL	B	401	6/6	0.78	0.19	45,68,85,89	14
4	A1AVS	A	404	16/16	0.79	0.20	40,62,91,93	25
4	A1AVS	B	404	16/16	0.85	0.18	31,50,66,76	25
2	FMN	A	401	31/31	0.96	0.07	34,40,49,55	0
2	FMN	B	402	31/31	0.97	0.07	23,29,38,38	0

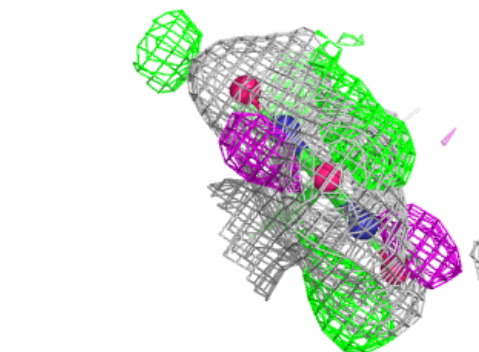
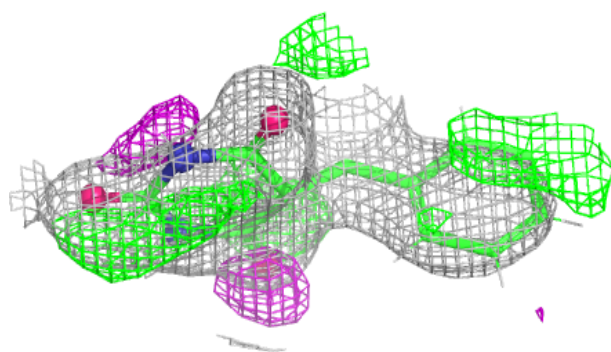
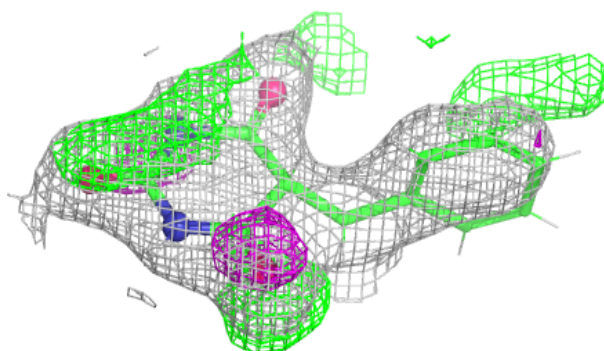
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around A1AVS A 404:

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

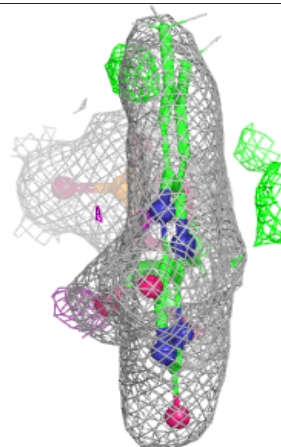
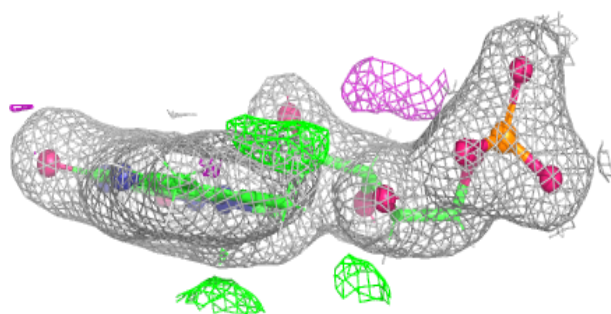
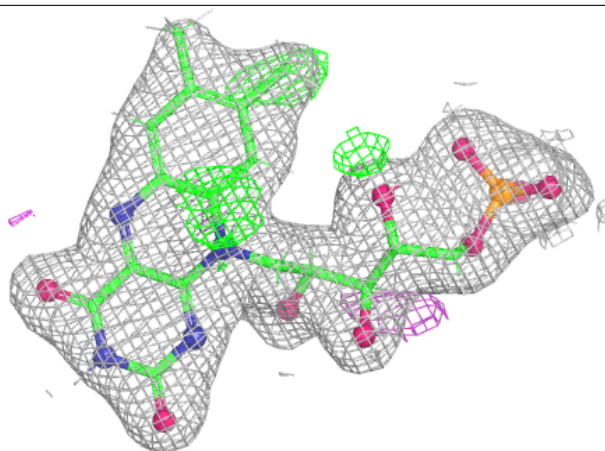
**Electron density around A1AVS B 404:**

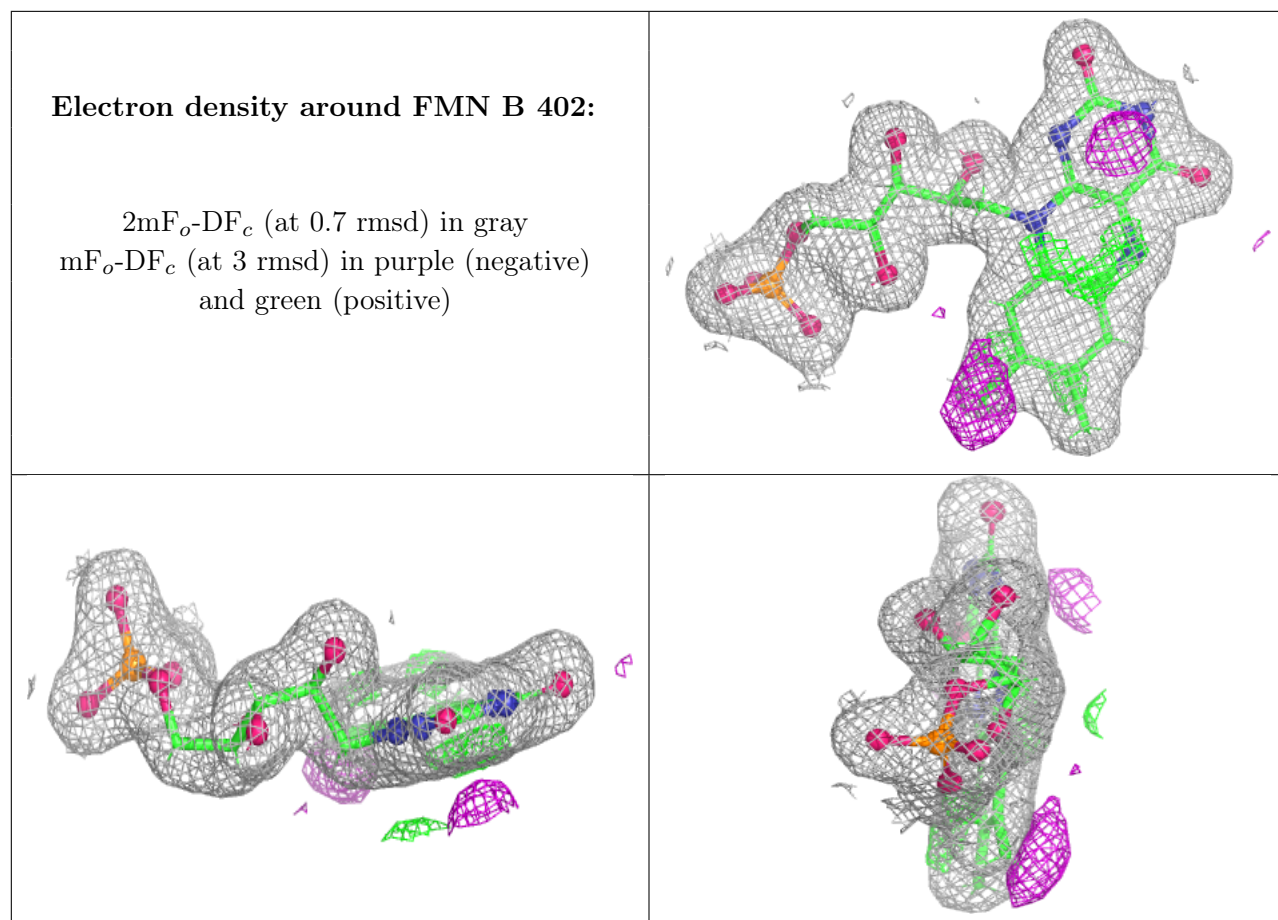
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around FMN A 401:

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





6.5 Other polymers ⓘ

There are no such residues in this entry.