



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 10:25 PM UTC

PDB ID : 6I4B / pdb_00006i4b
Title : Plasmodium falciparum dihydroorotate dehydrogenase (DHODH) co-crystallized with 3-Hydroxy-1-methyl-5-((3-(trifluoromethyl)phenoxy)methyl)-1H-pyrazole-4-carboxylic acid
Authors : Goyal, P.; Sainas, S.; Pippione, A.C.; Boschi, D.; Al-Kadaraghi, S.
Deposited on : 2018-11-09
Resolution : 1.98 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)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

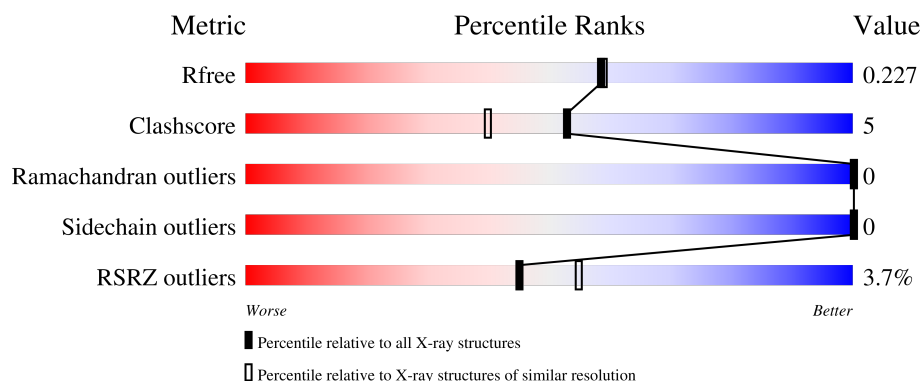
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

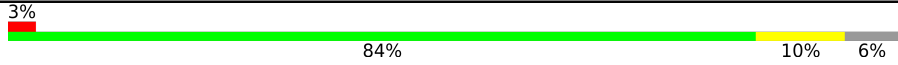
The reported resolution of this entry is 1.98 Å.

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}	180053	1506 (1.98-1.98)
Clashscore	190562	1534 (1.98-1.98)
Ramachandran outliers	187476	1518 (1.98-1.98)
Sidechain outliers	187428	1518 (1.98-1.98)
RSRZ outliers	180081	1506 (1.98-1.98)

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	405	
1	B	405	

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	ORO	A	602	-	X	-	-
3	ORO	B	602	-	X	-	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6422 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 Dihydroorotate dehydrogenase (quinone), mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	381	Total	C	N	O	S	0	1	0
			3029	1936	506	571	16			
1	B	374	Total	C	N	O	S	0	2	0
			2973	1903	497	558	15			

There are 106 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	135	MET	-	initiating methionine	UNP Q08210
A	136	HIS	-	expression tag	UNP Q08210
A	137	HIS	-	expression tag	UNP Q08210
A	138	HIS	-	expression tag	UNP Q08210
A	139	HIS	-	expression tag	UNP Q08210
A	140	HIS	-	expression tag	UNP Q08210
A	141	HIS	-	expression tag	UNP Q08210
A	142	SER	-	expression tag	UNP Q08210
A	143	SER	-	expression tag	UNP Q08210
A	144	GLY	-	expression tag	UNP Q08210
A	145	VAL	-	expression tag	UNP Q08210
A	146	ASP	-	expression tag	UNP Q08210
A	147	LEU	-	expression tag	UNP Q08210
A	148	GLY	-	expression tag	UNP Q08210
A	149	THR	-	expression tag	UNP Q08210
A	150	GLU	-	expression tag	UNP Q08210
A	151	ASN	-	expression tag	UNP Q08210
A	152	LEU	-	expression tag	UNP Q08210
A	153	TYR	-	expression tag	UNP Q08210
A	154	PHE	-	expression tag	UNP Q08210
A	155	GLN	-	expression tag	UNP Q08210
A	156	SER	-	expression tag	UNP Q08210
A	157	MET	-	expression tag	UNP Q08210
A	?	-	SER	deletion	UNP Q08210
A	?	-	THR	deletion	UNP Q08210

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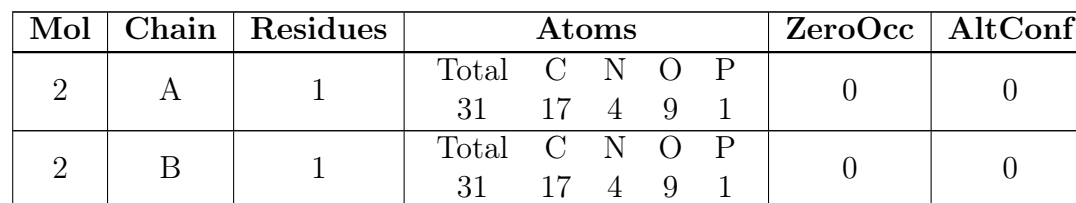
Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	TYR	deletion	UNP Q08210
A	?	-	ASN	deletion	UNP Q08210
A	?	-	GLU	deletion	UNP Q08210
A	?	-	ASP	deletion	UNP Q08210
A	?	-	ASN	deletion	UNP Q08210
A	?	-	LYS	deletion	UNP Q08210
A	?	-	ILE	deletion	UNP Q08210
A	?	-	VAL	deletion	UNP Q08210
A	?	-	GLU	deletion	UNP Q08210
A	?	-	LYS	deletion	UNP Q08210
A	?	-	LYS	deletion	UNP Q08210
A	?	-	ASN	deletion	UNP Q08210
A	?	-	ASN	deletion	UNP Q08210
A	?	-	PHE	deletion	UNP Q08210
A	?	-	ASN	deletion	UNP Q08210
A	?	-	LYS	deletion	UNP Q08210
A	?	-	ASN	deletion	UNP Q08210
A	?	-	ASN	deletion	UNP Q08210
A	?	-	SER	deletion	UNP Q08210
A	?	-	HIS	deletion	UNP Q08210
A	?	-	MET	deletion	UNP Q08210
A	?	-	MET	deletion	UNP Q08210
A	?	-	LYS	deletion	UNP Q08210
A	?	-	ASP	deletion	UNP Q08210
A	?	-	ALA	deletion	UNP Q08210
A	?	-	LYS	deletion	UNP Q08210
A	?	-	ASP	deletion	UNP Q08210
A	?	-	ASN	deletion	UNP Q08210
B	135	MET	-	initiating methionine	UNP Q08210
B	136	HIS	-	expression tag	UNP Q08210
B	137	HIS	-	expression tag	UNP Q08210
B	138	HIS	-	expression tag	UNP Q08210
B	139	HIS	-	expression tag	UNP Q08210
B	140	HIS	-	expression tag	UNP Q08210
B	141	HIS	-	expression tag	UNP Q08210
B	142	SER	-	expression tag	UNP Q08210
B	143	SER	-	expression tag	UNP Q08210
B	144	GLY	-	expression tag	UNP Q08210
B	145	VAL	-	expression tag	UNP Q08210
B	146	ASP	-	expression tag	UNP Q08210
B	147	LEU	-	expression tag	UNP Q08210
B	148	GLY	-	expression tag	UNP Q08210

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Chain	Residue	Modelled	Actual	Comment	Reference
B	149	THR	-	expression tag	UNP Q08210
B	150	GLU	-	expression tag	UNP Q08210
B	151	ASN	-	expression tag	UNP Q08210
B	152	LEU	-	expression tag	UNP Q08210
B	153	TYR	-	expression tag	UNP Q08210
B	154	PHE	-	expression tag	UNP Q08210
B	155	GLN	-	expression tag	UNP Q08210
B	156	SER	-	expression tag	UNP Q08210
B	157	MET	-	expression tag	UNP Q08210
B	?	-	SER	deletion	UNP Q08210
B	?	-	THR	deletion	UNP Q08210
B	?	-	TYR	deletion	UNP Q08210
B	?	-	ASN	deletion	UNP Q08210
B	?	-	GLU	deletion	UNP Q08210
B	?	-	ASP	deletion	UNP Q08210
B	?	-	ASN	deletion	UNP Q08210
B	?	-	LYS	deletion	UNP Q08210
B	?	-	ILE	deletion	UNP Q08210
B	?	-	VAL	deletion	UNP Q08210
B	?	-	GLU	deletion	UNP Q08210
B	?	-	LYS	deletion	UNP Q08210
B	?	-	LYS	deletion	UNP Q08210
B	?	-	ASN	deletion	UNP Q08210
B	?	-	ASN	deletion	UNP Q08210
B	?	-	PHE	deletion	UNP Q08210
B	?	-	ASN	deletion	UNP Q08210
B	?	-	LYS	deletion	UNP Q08210
B	?	-	ASN	deletion	UNP Q08210
B	?	-	ASN	deletion	UNP Q08210
B	?	-	SER	deletion	UNP Q08210
B	?	-	HIS	deletion	UNP Q08210
B	?	-	MET	deletion	UNP Q08210
B	?	-	MET	deletion	UNP Q08210
B	?	-	LYS	deletion	UNP Q08210
B	?	-	ASP	deletion	UNP Q08210
B	?	-	ALA	deletion	UNP Q08210
B	?	-	LYS	deletion	UNP Q08210
B	?	-	ASP	deletion	UNP Q08210
B	?	-	ASN	deletion	UNP Q08210

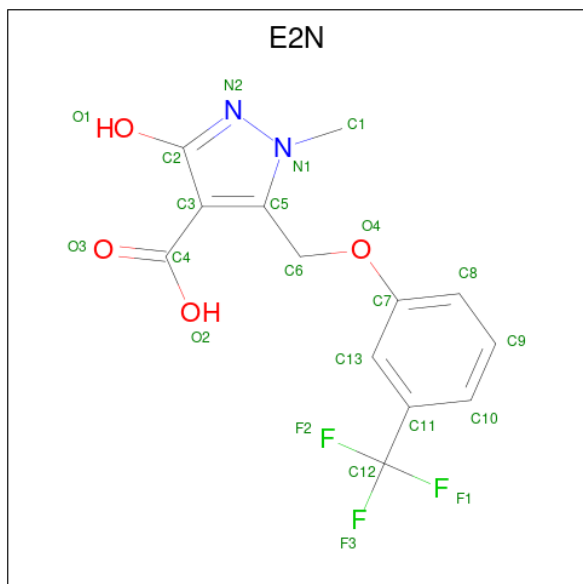
- Molecule 2 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: C₁₇H₂₁N₄O₉P).



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- Chemical structure of Orothione (ORO) is shown. The structure is a pyrimidine ring with a carboxylic acid group at position 2 and a thioamide group at position 4. The atoms are labeled as follows: N1 (blue), N3 (blue), C2 (green), C4 (green), C5 (green), C6 (green), O71 (green), O72 (green), O2 (green), and O4 (green). The carboxylic acid group is represented by a red HO group and a red O atom. The thioamide group is represented by a blue NH group and a red O atom.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total 11	C 5	N 2	O 4	0	0
3	B	1	Total 11	C 5	N 2	O 4	0	0

- Molecule 4 is 1-methyl-3-oxidanyl-5-[[3-(trifluoromethyl)phenoxy]methyl]pyrazole-4-carboxylic acid (CCD ID: E2N) (formula: $C_{13}H_{11}F_3N_2O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	F	N	O	0	0
			22	13	3	2	4		
4	B	1	Total	C	F	N	O	0	0
			22	13	3	2	4		

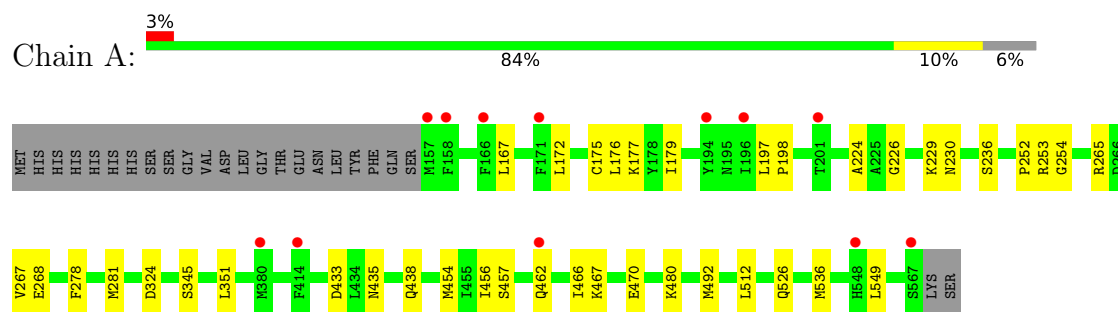
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	147	Total	O	0	0
			147	147		
5	B	145	Total	O	0	0
			145	145		

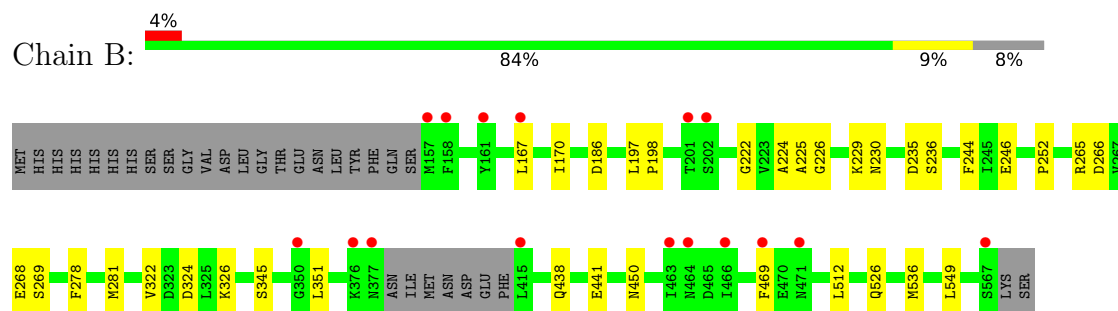
3 Residue-property plots [i](#)

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 (quinone), mitochondrial



- Molecule 1: Dihydroorotate dehydrogenase (quinone), mitochondrial



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	50.61Å 158.12Å 61.75Å 90.00° 105.67° 90.00°	Depositor
Resolution (Å)	48.73 – 1.98 48.73 – 1.98	Depositor EDS
% Data completeness (in resolution range)	99.2 (48.73-1.98) 99.1 (48.73-1.98)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.72 (at 1.98Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.192 , 0.226 0.194 , 0.227	Depositor DCC
R_{free} test set	3263 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	32.4	Xtriage
Anisotropy	0.321	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 42.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	6422	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.79% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ORO, FMN, E2N

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	0.25	0/3084	0.44	0/4152
1	B	0.27	0/3029	0.44	0/4077
All	All	0.26	0/6113	0.44	0/8229

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	3029	0	3066	35	0
1	B	2973	0	3023	27	0
2	A	31	0	19	1	0
2	B	31	0	19	1	0
3	A	11	0	3	2	0
3	B	11	0	3	2	0
4	A	22	0	0	1	0
4	B	22	0	0	1	0
5	A	147	0	0	1	0
5	B	145	0	0	1	0
All	All	6422	0	6133	61	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 5.

All (61) 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:230:ASN:HB3	1:A:281:MET:HE2	1.62	0.80
1:A:454:MET:HE2	1:A:456:ILE:HD11	1.67	0.74
1:B:198:PRO:HD2	1:B:536:MET:HE2	1.71	0.72
1:A:198:PRO:HD2	1:A:536:MET:HE2	1.75	0.68
1:B:197:LEU:HD22	1:B:536:MET:HE1	1.80	0.63
1:A:466:ILE:HD11	1:A:480:LYS:HD3	1.81	0.63
1:A:197:LEU:HD22	1:A:536:MET:HE1	1.85	0.59
1:B:230:ASN:HB3	1:B:281:MET:HE2	1.84	0.59
1:A:175:CYS:HA	1:A:179:ILE:HD13	1.85	0.59
1:A:230:ASN:CG	1:A:281:MET:HG3	2.29	0.58
1:B:230:ASN:CG	1:B:281:MET:HG3	2.29	0.57
1:A:512:LEU:HD12	1:A:549:LEU:HD21	1.88	0.56
1:A:172:LEU:C	1:A:172:LEU:HD13	2.32	0.54
1:B:345:SER:HB3	1:B:351:LEU:HD23	1.90	0.54
1:A:467:LYS:HA	1:A:470:GLU:HB2	1.90	0.52
1:B:224:ALA:HB2	1:B:526:GLN:HB3	1.91	0.52
1:A:278:PHE:CE2	3:A:602:ORO:H5	2.46	0.50
1:A:226:GLY:HA3	2:A:601:FMN:N5	2.26	0.50
1:A:197:LEU:HD12	1:A:236:SER:HB3	1.94	0.49
1:B:268:GLU:CD	1:B:268:GLU:H	2.20	0.49
1:B:278:PHE:CE1	3:B:602:ORO:H5	2.49	0.48
1:B:438:GLN:HA	1:B:441:GLU:HG2	1.95	0.48
1:A:433:ASP:HA	1:A:462:GLN:NE2	2.28	0.47
1:B:197:LEU:HD12	1:B:236:SER:HB3	1.96	0.47
1:A:252:PRO:HG2	1:A:324:ASP:CG	2.40	0.47
1:A:167:LEU:HD12	1:A:167:LEU:HA	1.79	0.46
1:A:549:LEU:HD12	1:A:549:LEU:HA	1.82	0.46
1:B:322:VAL:HG12	1:B:326:LYS:HE3	1.97	0.46
1:B:512:LEU:HD22	1:B:549:LEU:HD21	1.97	0.46
1:B:266:ASP:OD2	1:B:269:SER:OG	2.30	0.45
1:A:265:ARG:HD3	4:A:603:E2N:N2	2.32	0.45
1:B:265:ARG:HD3	4:B:603:E2N:N2	2.32	0.45
1:B:186:ASP:OD2	5:B:701:HOH:O	2.21	0.45
1:B:225:ALA:HA	1:B:246:GLU:O	2.17	0.45
1:A:172:LEU:HD13	1:A:176:LEU:HG	1.99	0.45
1:A:435:ASN:OD1	1:A:438:GLN:HG3	2.18	0.44
1:B:226:GLY:HA3	2:B:601:FMN:N5	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:278:PHE:HE2	3:A:602:ORO:H5	1.82	0.44
1:B:167:LEU:HD23	1:B:170:ILE:HD12	2.00	0.44
1:A:433:ASP:HA	1:A:462:GLN:HE21	1.83	0.43
1:A:512:LEU:HD12	1:A:549:LEU:CD2	2.49	0.43
1:A:177:LYS:HE2	1:A:267:VAL:HG21	2.01	0.42
1:A:456:ILE:HA	1:A:457:SER:HA	1.79	0.42
1:A:254:GLY:O	1:B:450:ASN:HB2	2.19	0.42
1:B:226:GLY:HA2	1:B:229:LYS:HG3	2.01	0.42
1:B:222:GLY:HA3	1:B:244:PHE:CE2	2.54	0.42
1:A:267:VAL:HG23	1:A:268:GLU:OE1	2.19	0.42
1:B:235:ASP:OD1	1:B:235:ASP:N	2.51	0.42
1:A:454:MET:HE1	1:A:492:MET:CE	2.49	0.42
1:B:278:PHE:HE1	3:B:602:ORO:H5	1.84	0.41
1:B:549:LEU:HA	1:B:549:LEU:HD12	1.79	0.41
1:A:172:LEU:HD13	1:A:172:LEU:O	2.20	0.41
1:A:226:GLY:HA2	1:A:229:LYS:HG3	2.02	0.41
1:B:252:PRO:HG2	1:B:324:ASP:CG	2.45	0.41
1:B:266:ASP:HB2	1:B:469:PHE:CE2	2.56	0.41
1:A:253:ARG:NH2	5:A:706:HOH:O	2.50	0.41
1:A:345:SER:HB3	1:A:351:LEU:HD23	2.03	0.40
1:A:224:ALA:HB2	1:A:526:GLN:HB3	2.01	0.40
1:B:230:ASN:OD1	1:B:281:MET:HG3	2.20	0.40
1:A:230:ASN:OD1	1:A:281:MET:HG3	2.21	0.40
1:A:454:MET:HE1	1:A:492:MET:HE3	2.04	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	380/405 (94%)	368 (97%)	12 (3%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	372/405 (92%)	363 (98%)	9 (2%)	0	100	100
All	All	752/810 (93%)	731 (97%)	21 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	339/360 (94%)	339 (100%)	0	100	100
1	B	333/360 (92%)	333 (100%)	0	100	100
All	All	672/720 (93%)	672 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	289	ASN
1	A	378	ASN
1	A	494	ASN
1	B	497	ASN
1	B	499	GLN
1	B	541	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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
2	FMN	B	601	-	33,33,33	2.80	10 (30%)	48,50,50	1.76	8 (16%)
4	E2N	A	603	-	23,23,23	1.43	4 (17%)	27,34,34	1.47	4 (14%)
3	ORO	A	602	-	11,11,11	3.13	6 (54%)	14,15,15	2.37	5 (35%)
2	FMN	A	601	-	33,33,33	2.76	10 (30%)	48,50,50	1.62	8 (16%)
3	ORO	B	602	-	11,11,11	3.05	6 (54%)	14,15,15	2.61	7 (50%)
4	E2N	B	603	-	23,23,23	1.40	4 (17%)	27,34,34	1.62	5 (18%)

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	B	601	-	-	1/18/18/18	0/3/3/3
4	E2N	A	603	-	-	0/15/15/15	0/2/2/2
3	ORO	A	602	-	-	4/4/4/4	0/1/1/1
2	FMN	A	601	-	-	1/18/18/18	0/3/3/3
3	ORO	B	602	-	-	3/4/4/4	0/1/1/1
4	E2N	B	603	-	-	0/15/15/15	0/2/2/2

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	FMN	C4A-N5	7.04	1.45	1.30
2	A	601	FMN	C4A-N5	6.94	1.45	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	FMN	C10-N1	6.62	1.46	1.33
2	B	601	FMN	C10-N1	6.45	1.46	1.33
2	A	601	FMN	C5A-N5	5.61	1.49	1.39
2	B	601	FMN	C5A-N5	5.40	1.49	1.39
2	B	601	FMN	C9A-N10	5.25	1.50	1.41
2	B	601	FMN	C2-N1	5.24	1.48	1.36
2	A	601	FMN	C9A-N10	5.20	1.50	1.41
3	A	602	ORO	C2-N1	5.20	1.46	1.37
3	B	602	ORO	C2-N1	5.13	1.45	1.37
2	A	601	FMN	C2-N1	5.04	1.48	1.36
3	B	602	ORO	C5-C4	4.94	1.53	1.42
3	A	602	ORO	C5-C4	4.82	1.52	1.42
3	A	602	ORO	C6-N1	4.67	1.48	1.38
3	B	602	ORO	C6-N1	4.42	1.48	1.38
2	B	601	FMN	C2-N3	4.28	1.48	1.39
2	A	601	FMN	C2-N3	4.00	1.47	1.39
2	B	601	FMN	C10-N10	3.88	1.45	1.37
2	B	601	FMN	C4-N3	3.60	1.45	1.38
3	A	602	ORO	C2-N3	3.53	1.43	1.37
2	A	601	FMN	C10-N10	3.48	1.44	1.37
2	A	601	FMN	C4-N3	3.32	1.45	1.38
2	B	601	FMN	O2-C2	-3.05	1.18	1.24
2	A	601	FMN	O2-C2	-3.01	1.18	1.24
3	B	602	ORO	C2-N3	3.00	1.42	1.37
3	B	602	ORO	O4-C4	-2.61	1.19	1.24
3	A	602	ORO	O4-C4	-2.55	1.19	1.24
4	A	603	E2N	C6-C5	2.54	1.53	1.49
2	B	601	FMN	O4-C4	-2.52	1.18	1.23
2	A	601	FMN	O4-C4	-2.48	1.18	1.23
4	A	603	E2N	C5-N1	-2.41	1.31	1.35
4	B	603	E2N	C6-C5	2.41	1.52	1.49
4	B	603	E2N	C3-C4	2.38	1.53	1.48
3	A	602	ORO	C4-N3	2.33	1.42	1.38
4	B	603	E2N	C5-N1	-2.33	1.31	1.35
4	A	603	E2N	C3-C4	2.31	1.53	1.48
3	B	602	ORO	O2-C2	-2.17	1.18	1.23
4	B	603	E2N	O1-C2	2.12	1.40	1.33
4	A	603	E2N	O1-C2	2.12	1.40	1.33

All (37) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	FMN	C7M-C7-C6	-6.58	107.97	119.57
2	A	601	FMN	C7M-C7-C6	-5.86	109.25	119.57
2	B	601	FMN	C7M-C7-C8	5.53	132.05	120.76
3	A	602	ORO	C4-N3-C2	-5.12	120.58	125.55
3	B	602	ORO	C4-N3-C2	-4.95	120.75	125.55
2	A	601	FMN	C7M-C7-C8	4.84	130.64	120.76
3	A	602	ORO	O4-C4-C5	-4.14	119.74	125.46
3	B	602	ORO	O4-C4-C5	-3.81	120.20	125.46
4	B	603	E2N	C1-N1-N2	3.79	124.95	119.29
4	A	603	E2N	C1-N1-N2	3.75	124.90	119.29
3	B	602	ORO	C6-N1-C2	-3.51	118.90	122.65
3	B	602	ORO	O72-C7-C6	3.47	121.75	114.27
3	A	602	ORO	C5-C4-N3	3.40	119.46	115.24
2	B	601	FMN	C4-N3-C2	-3.30	119.79	125.64
3	B	602	ORO	C5-C4-N3	3.24	119.27	115.24
3	A	602	ORO	C6-N1-C2	-3.10	119.33	122.65
2	A	601	FMN	C4A-C10-N10	2.82	120.53	116.48
2	B	601	FMN	C4A-C10-N10	2.78	120.46	116.48
2	A	601	FMN	C5A-C9A-N10	2.73	120.44	117.97
4	B	603	E2N	F3-C12-C11	-2.72	107.07	112.90
3	B	602	ORO	N3-C2-N1	2.70	119.99	115.74
3	B	602	ORO	O71-C7-C6	-2.55	115.83	121.01
2	B	601	FMN	C4A-C4-N3	2.54	119.72	113.25
4	B	603	E2N	O1-C2-N2	2.50	127.02	122.94
4	A	603	E2N	O1-C2-N2	2.49	127.01	122.94
2	B	601	FMN	C5A-C9A-N10	2.48	120.21	117.97
2	A	601	FMN	C4-N3-C2	-2.47	121.25	125.64
3	A	602	ORO	N3-C2-N1	2.45	119.58	115.74
2	B	601	FMN	C10-C4A-N5	-2.40	119.91	124.81
2	A	601	FMN	C4A-C4-N3	2.34	119.20	113.25
4	A	603	E2N	C4-C3-C2	2.28	125.99	121.80
2	A	601	FMN	C10-C4A-N5	-2.26	120.20	124.81
4	B	603	E2N	C4-C3-C2	2.24	125.92	121.80
2	B	601	FMN	O4-C4-C4A	-2.17	120.80	126.53
4	B	603	E2N	F2-C12-C11	-2.13	108.34	112.90
2	A	601	FMN	C9A-C5A-N5	-2.06	120.27	122.45
4	A	603	E2N	F3-C12-C11	-2.01	108.59	112.90

There are no chirality outliers.

All (9) torsion outliers are listed below:

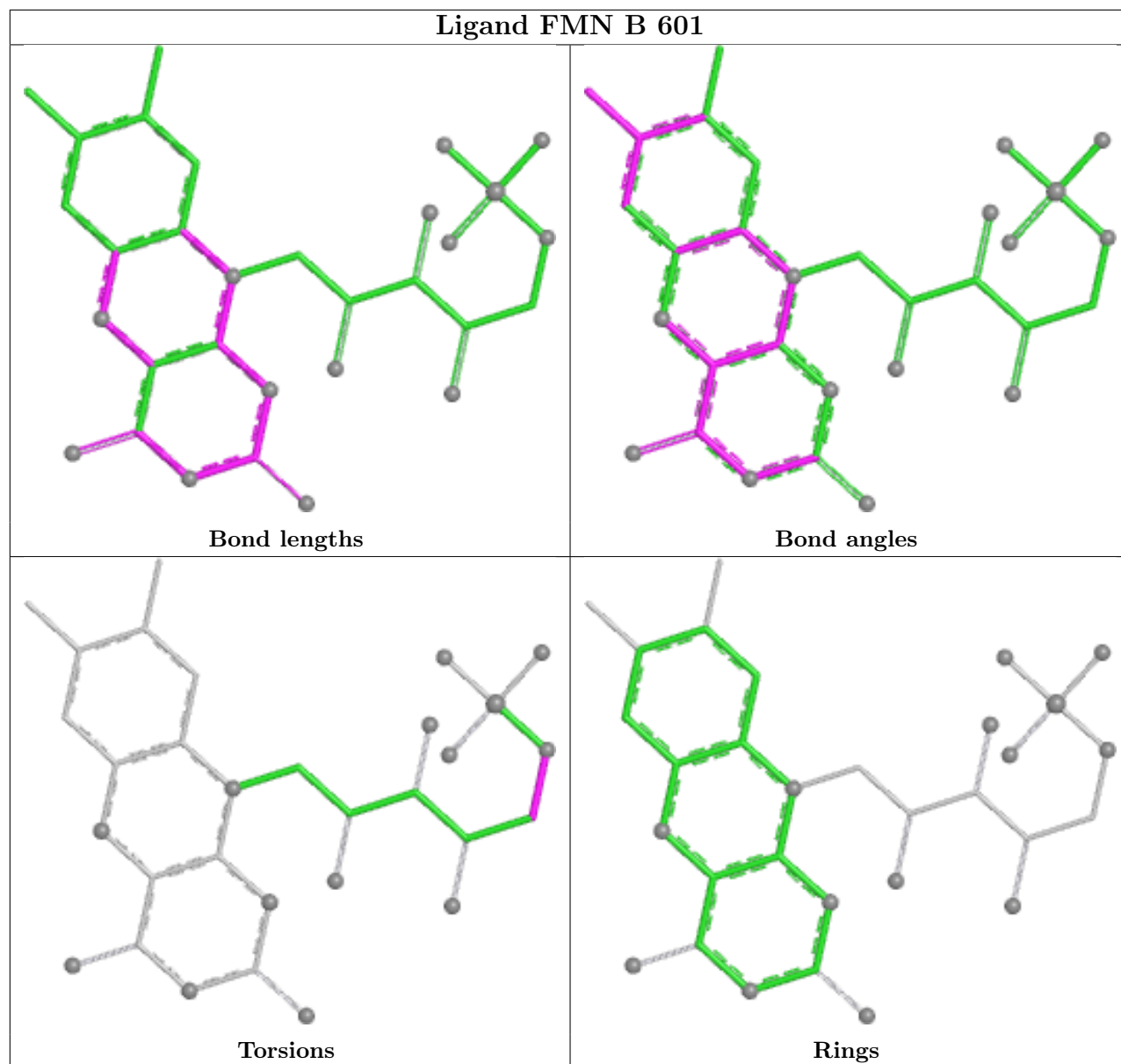
Mol	Chain	Res	Type	Atoms
3	A	602	ORO	N1-C6-C7-O71
3	A	602	ORO	N1-C6-C7-O72
3	A	602	ORO	C5-C6-C7-O71
3	A	602	ORO	C5-C6-C7-O72
3	B	602	ORO	N1-C6-C7-O71
3	B	602	ORO	N1-C6-C7-O72
2	B	601	FMN	C4'-C5'-O5'-P
2	A	601	FMN	C4'-C5'-O5'-P
3	B	602	ORO	C5-C6-C7-O72

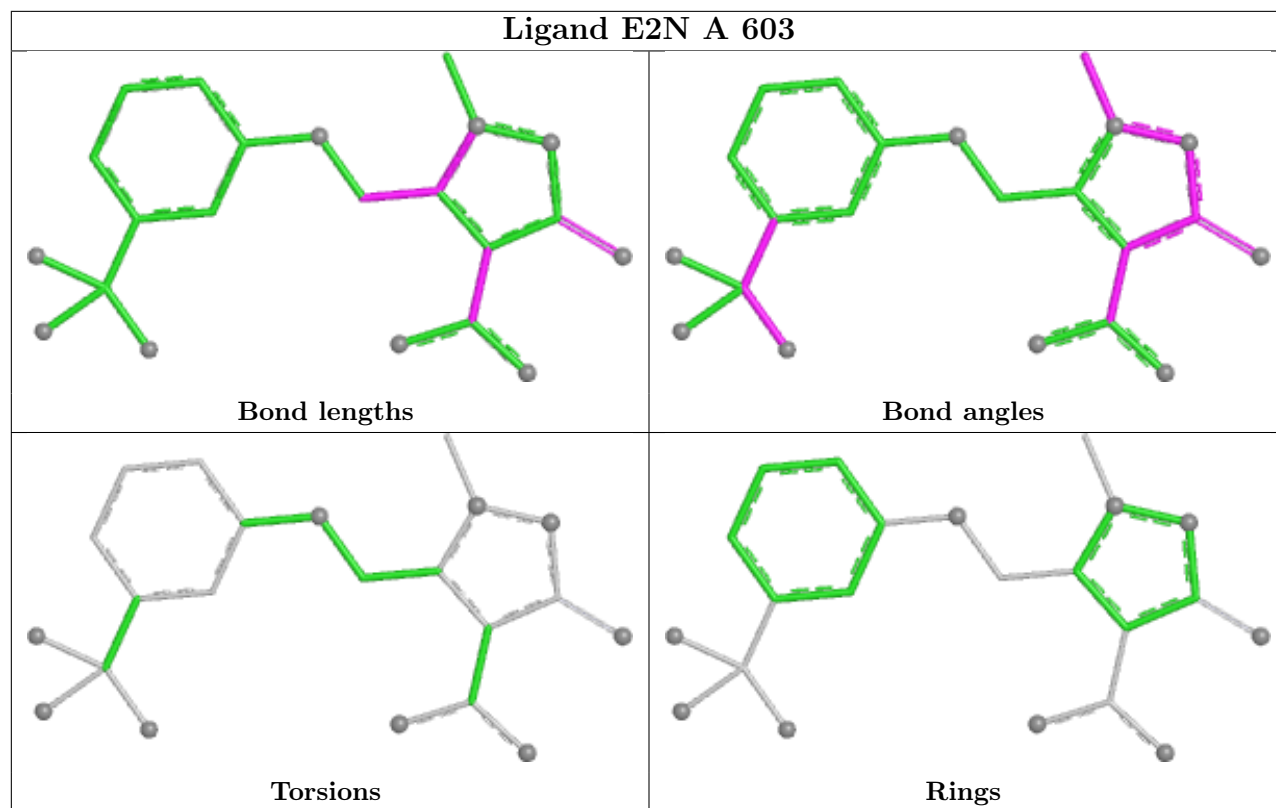
There are no ring outliers.

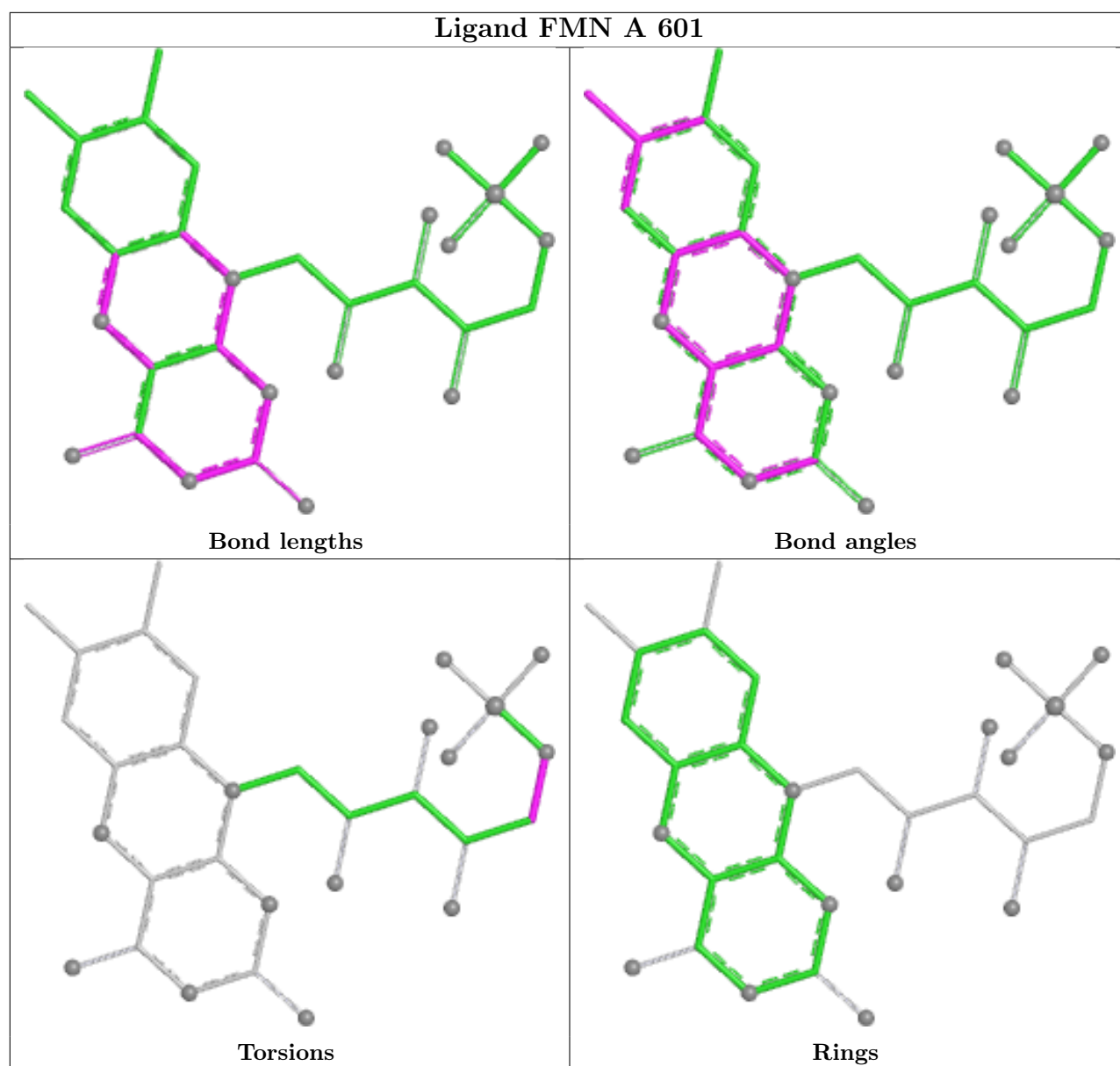
6 monomers are involved in 8 short contacts:

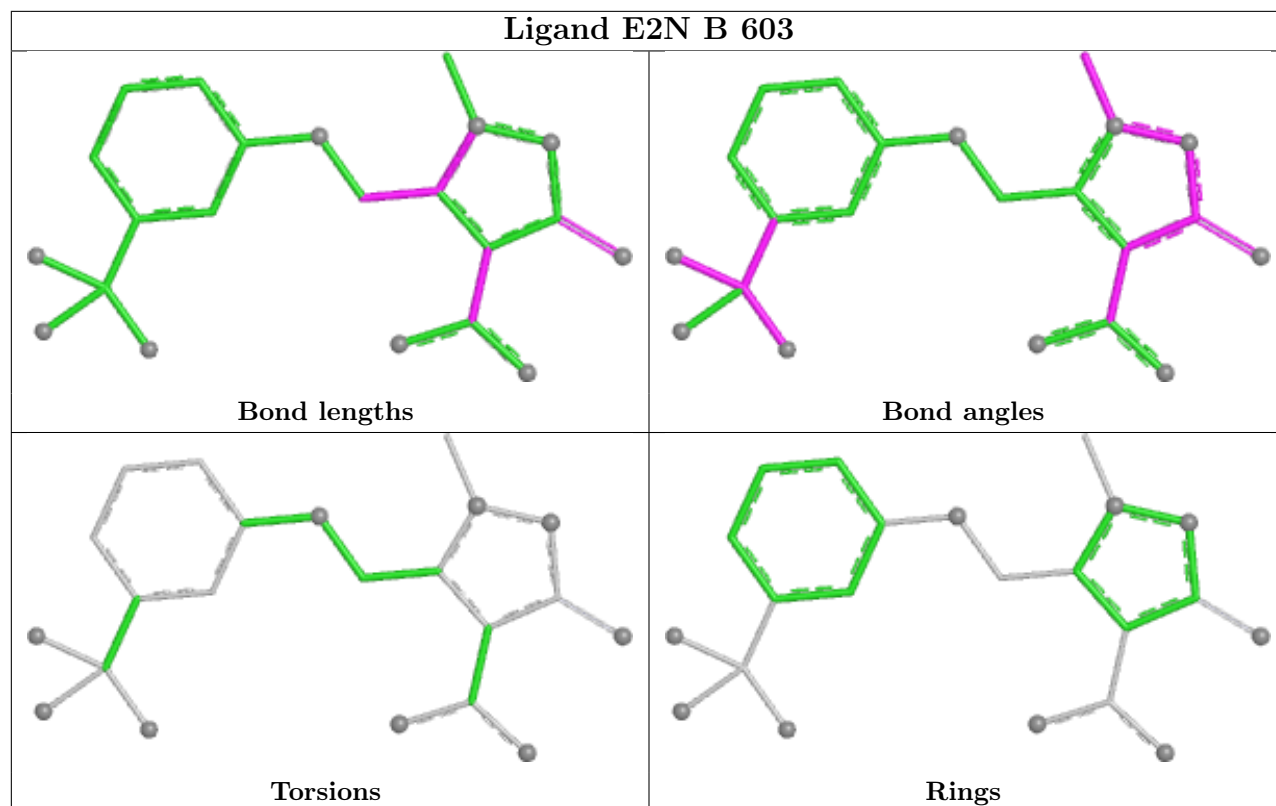
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	601	FMN	1	0
4	A	603	E2N	1	0
3	A	602	ORO	2	0
2	A	601	FMN	1	0
3	B	602	ORO	2	0
4	B	603	E2N	1	0

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

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	381/405 (94%)	0.27	12 (3%)	51 61	28, 44, 74, 105	1 (0%)
1	B	374/405 (92%)	0.28	16 (4%)	40 49	20, 45, 80, 117	2 (0%)
All	All	755/810 (93%)	0.28	28 (3%)	45 55	20, 45, 77, 117	3 (0%)

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	415	LEU	4.3
1	B	157	MET	3.7
1	B	201	THR	3.6
1	B	469	PHE	3.5
1	A	157	MET	3.4
1	B	158	PHE	3.2
1	A	567	SER	3.1
1	A	158	PHE	3.0
1	A	414	PHE	2.8
1	A	201	THR	2.8
1	B	376	LYS	2.7
1	A	548	HIS	2.5
1	A	380	MET	2.5
1	A	194	TYR	2.5
1	B	161	TYR	2.4
1	A	166	PHE	2.4
1	A	171	PHE	2.4
1	B	463	ILE	2.4
1	B	377	ASN	2.3
1	B	464	ASN	2.3
1	A	462	GLN	2.2
1	B	466	ILE	2.2
1	B	167	LEU	2.2
1	B	567	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	196	ILE	2.1
1	B	350	GLY	2.1
1	B	471	ASN	2.1
1	B	202	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](#)

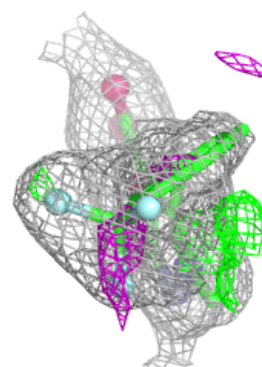
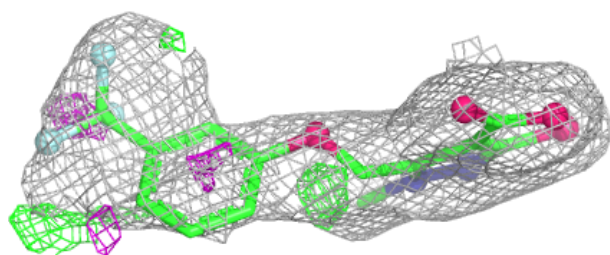
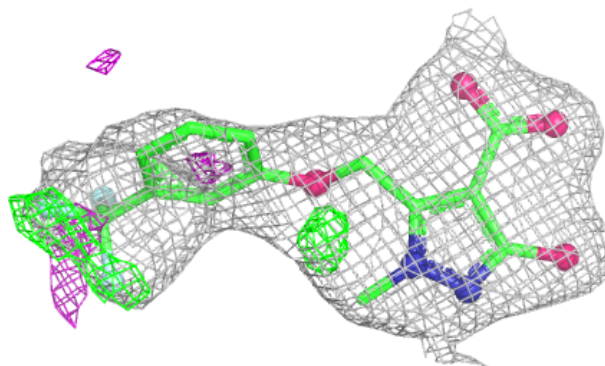
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	E2N	B	603	22/22	0.81	0.15	51,66,86,87	0
4	E2N	A	603	22/22	0.82	0.17	58,72,93,94	0
3	ORO	B	602	11/11	0.92	0.08	34,37,40,40	0
3	ORO	A	602	11/11	0.93	0.07	31,35,37,37	0
2	FMN	B	601	31/31	0.94	0.08	31,34,37,40	0
2	FMN	A	601	31/31	0.95	0.08	27,32,34,34	0

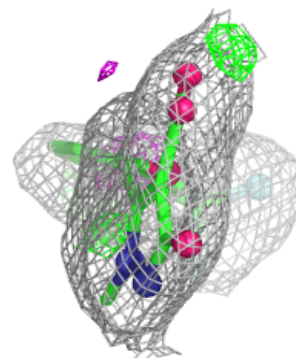
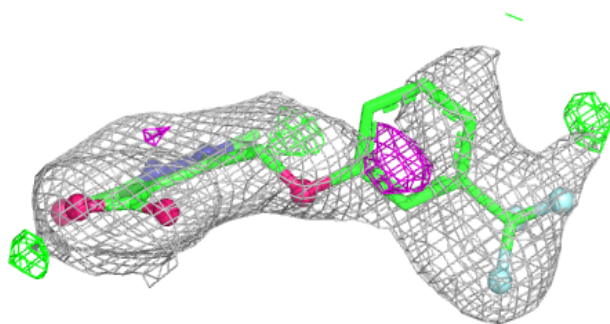
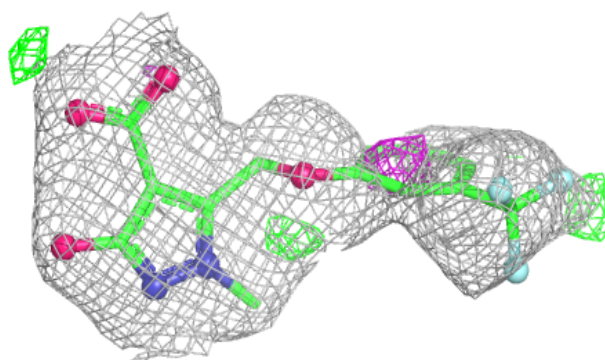
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around E2N B 603:

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

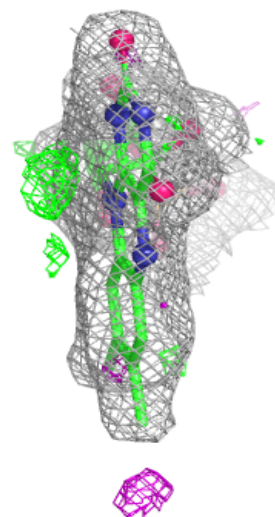
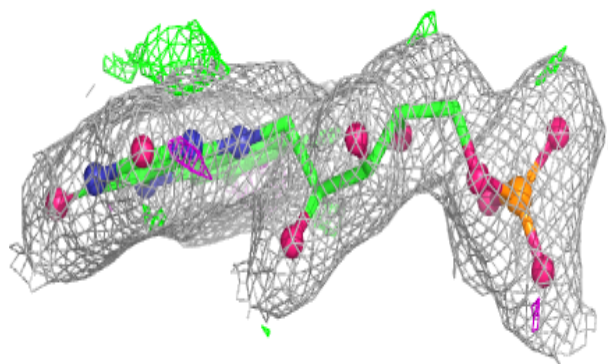
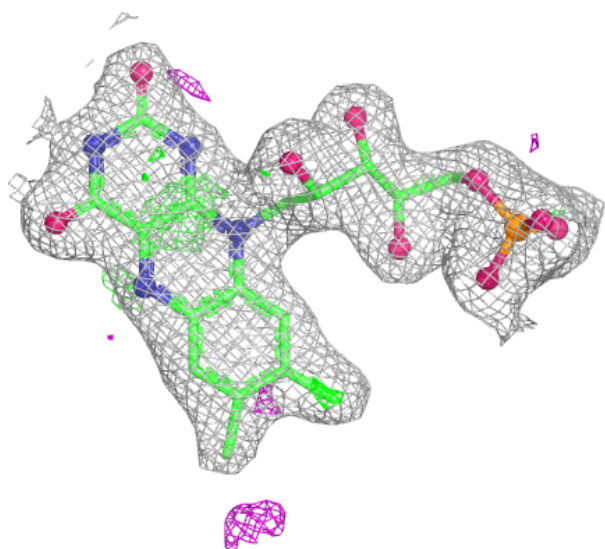
**Electron density around E2N A 603:**

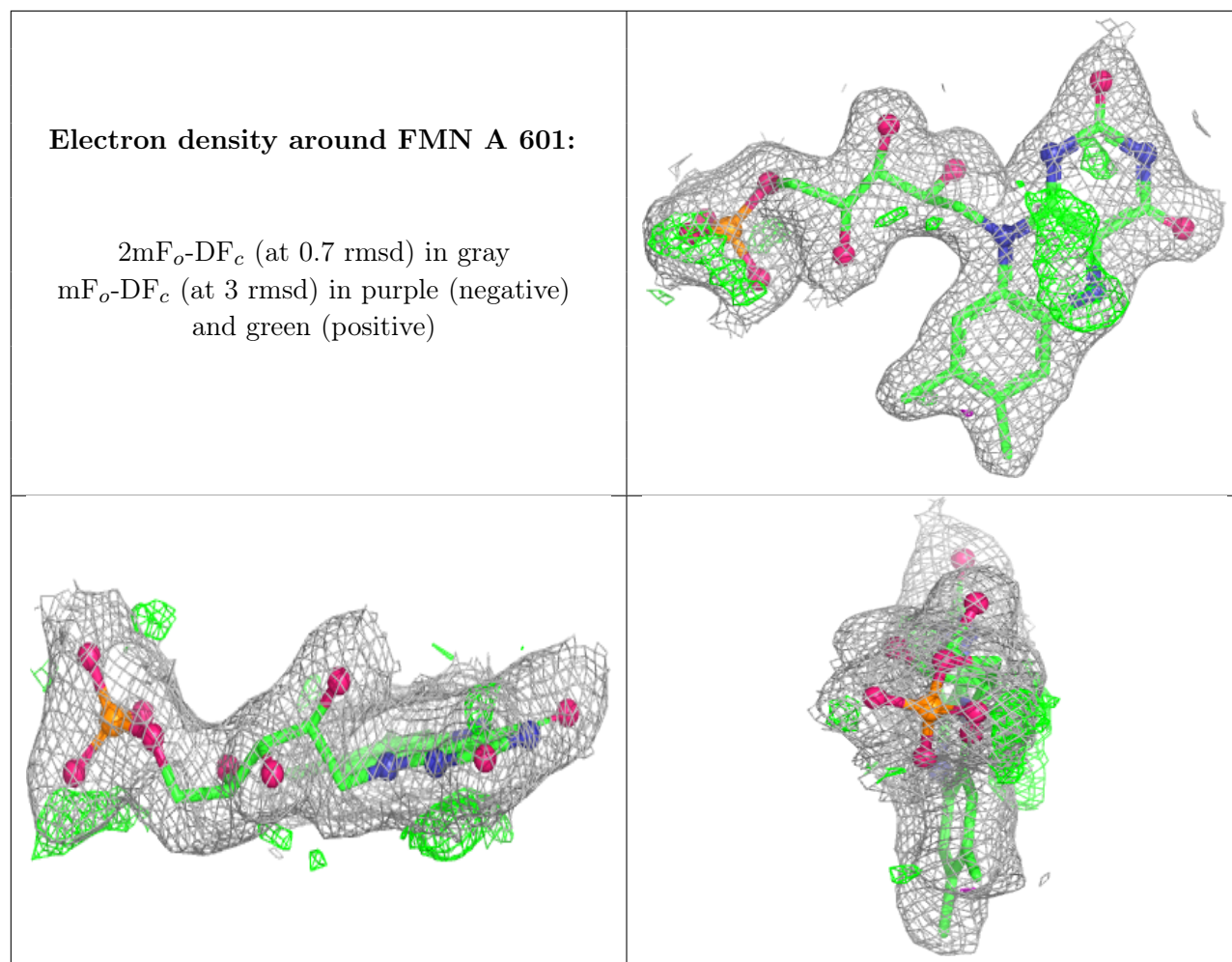
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around FMN B 601:

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





6.5 Other polymers [i](#)

There are no such residues in this entry.