



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 11:13 PM UTC

PDB ID : 4CQ9 / pdb_00004cq9
Title : Plasmodium falciparum dihydroorotate dehydrogenase (DHODH) in complex with IDI-6253
Authors : Rowland, P.
Deposited on : 2014-02-12
Resolution : 2.72 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

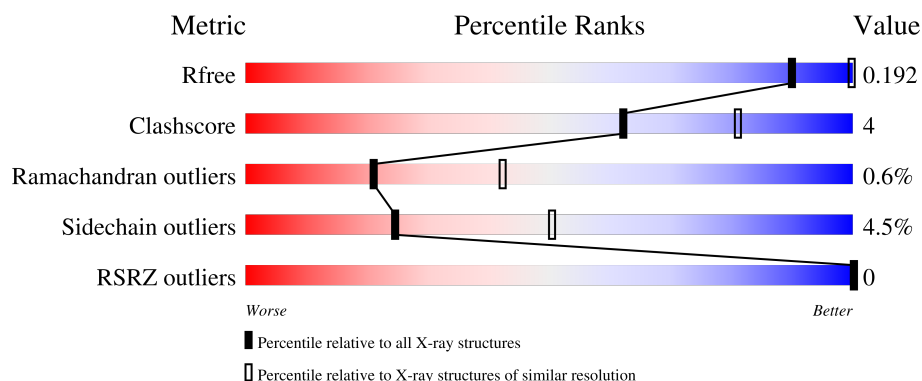
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.72 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	4348 (2.74-2.70)
Clashscore	190562	4665 (2.74-2.70)
Ramachandran outliers	187476	4584 (2.74-2.70)
Sidechain outliers	187428	4585 (2.74-2.70)
RSRZ outliers	180081	4348 (2.74-2.70)

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	401	 74% 16% • 8%
1	B	401	 75% 15% • 8%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6305 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	367	Total	C	N	O	S	0	0	0
			2902	1855	489	544	14			
1	B	367	Total	C	N	O	S	0	0	0
			2902	1855	489	544	14			

There are 38 discrepancies between the modelled and reference sequences:

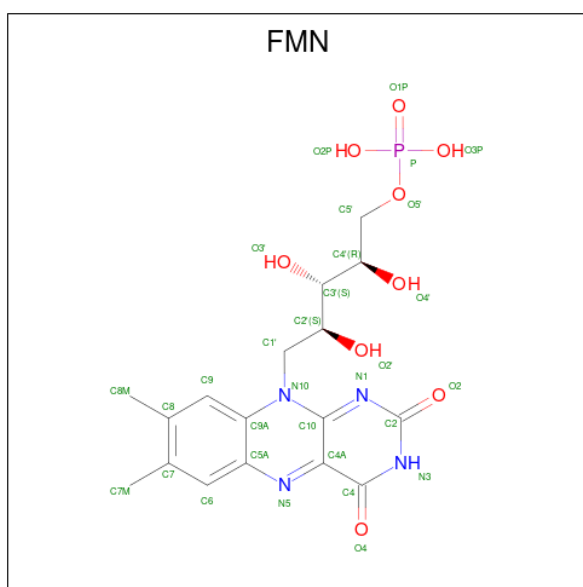
Chain	Residue	Modelled	Actual	Comment	Reference
A	139	MET	-	expression tag	UNP Q54A96
A	140	GLY	-	expression tag	UNP Q54A96
A	141	HIS	-	expression tag	UNP Q54A96
A	142	HIS	-	expression tag	UNP Q54A96
A	143	HIS	-	expression tag	UNP Q54A96
A	144	HIS	-	expression tag	UNP Q54A96
A	145	HIS	-	expression tag	UNP Q54A96
A	146	HIS	-	expression tag	UNP Q54A96
A	147	ALA	-	expression tag	UNP Q54A96
A	148	GLU	-	expression tag	UNP Q54A96
A	149	ASN	-	expression tag	UNP Q54A96
A	150	LEU	-	expression tag	UNP Q54A96
A	151	TYR	-	expression tag	UNP Q54A96
A	152	PHE	-	expression tag	UNP Q54A96
A	153	GLN	-	expression tag	UNP Q54A96
A	154	GLY	-	expression tag	UNP Q54A96
A	155	ALA	-	expression tag	UNP Q54A96
A	156	ASP	-	expression tag	UNP Q54A96
A	157	PRO	-	expression tag	UNP Q54A96
B	139	MET	-	expression tag	UNP Q54A96
B	140	GLY	-	expression tag	UNP Q54A96
B	141	HIS	-	expression tag	UNP Q54A96
B	142	HIS	-	expression tag	UNP Q54A96
B	143	HIS	-	expression tag	UNP Q54A96
B	144	HIS	-	expression tag	UNP Q54A96

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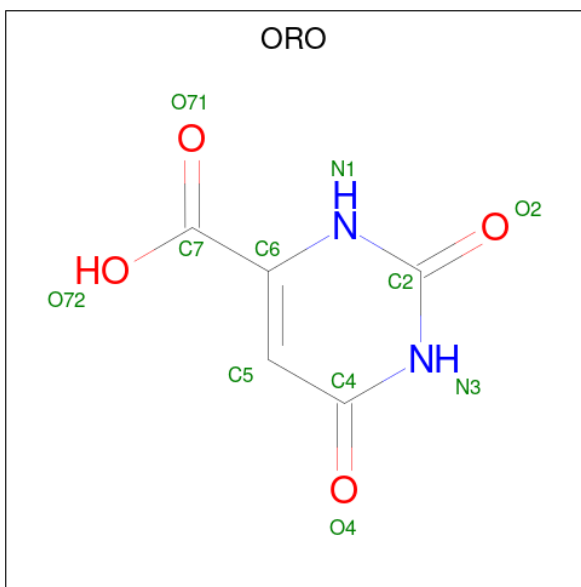
Chain	Residue	Modelled	Actual	Comment	Reference
B	145	HIS	-	expression tag	UNP Q54A96
B	146	HIS	-	expression tag	UNP Q54A96
B	147	ALA	-	expression tag	UNP Q54A96
B	148	GLU	-	expression tag	UNP Q54A96
B	149	ASN	-	expression tag	UNP Q54A96
B	150	LEU	-	expression tag	UNP Q54A96
B	151	TYR	-	expression tag	UNP Q54A96
B	152	PHE	-	expression tag	UNP Q54A96
B	153	GLN	-	expression tag	UNP Q54A96
B	154	GLY	-	expression tag	UNP Q54A96
B	155	ALA	-	expression tag	UNP Q54A96
B	156	ASP	-	expression tag	UNP Q54A96
B	157	PRO	-	expression tag	UNP Q54A96

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



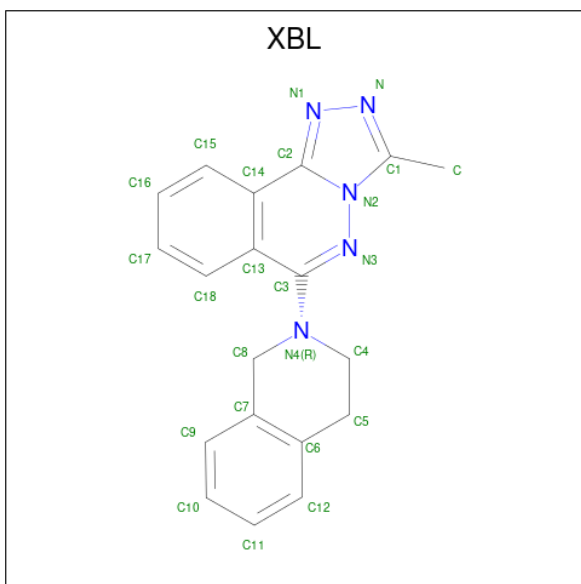
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	B	1	Total	C	N	O	P	0	0
			31	17	4	9	1		

- Molecule 3 is OROTIC ACID (CCD ID: ORO) (formula: $C_5H_4N_2O_4$).



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

- Molecule 4 is 6-(3,4-dihydroisoquinolin-2(1H)-yl)-3-methyl-[1,2,4]triazolo[3,4-a]phthalazine (CCD ID: XBL) (formula: C₁₉H₁₇N₅).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N		0	0
			24	19	5			

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	N	0	0
			24	19	5		

- Molecule 5 is water.

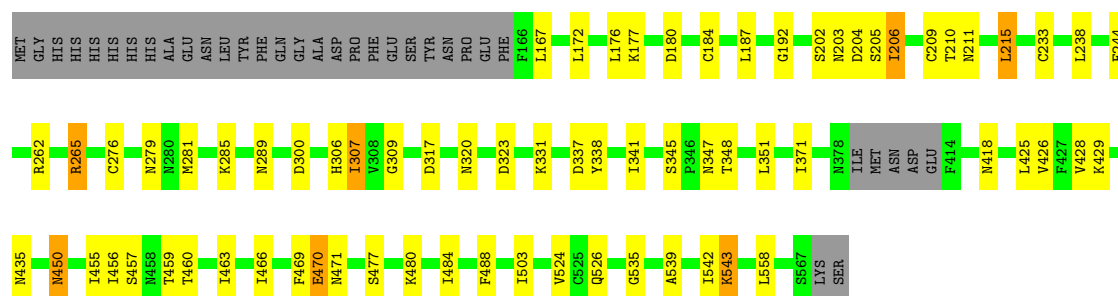
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	192	Total	O	0	0
			192	192		
5	B	177	Total	O	0	0
			177	177		

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.

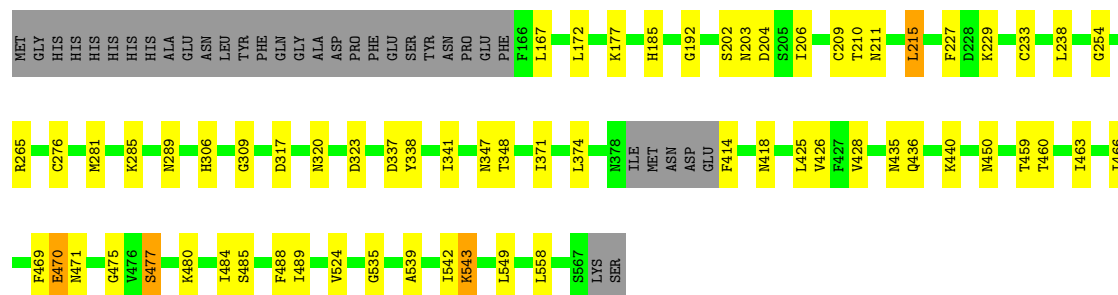
• Molecule 1: DIHYDROOROTATE DEHYDROGENASE

Chain A: 



• Molecule 1: DIHYDROOROTATE DEHYDROGENASE

Chain B: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	53.76Å 135.44Å 67.87Å 90.00° 89.64° 90.00°	Depositor
Resolution (Å)	49.97 – 2.72 49.97 – 2.72	Depositor EDS
% Data completeness (in resolution range)	84.0 (49.97-2.72) 83.1 (49.97-2.72)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.23 (at 2.73Å)	Xtriage
Refinement program	BUSTER 2.11.4	Depositor
R, R_{free}	0.194 , 0.268 0.162 , 0.192	Depositor DCC
R_{free} test set	888 reflections (4.05%)	wwPDB-VP
Wilson B-factor (Å ²)	47.6	Xtriage
Anisotropy	0.652	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 53.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.430 for h,-k,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	6305	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.18% 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: FMN, ORO, XBL

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	0.86	0/2949	1.44	22/3968 (0.6%)
1	B	0.87	0/2949	1.45	23/3968 (0.6%)
All	All	0.87	0/5898	1.44	45/7936 (0.6%)

There are no bond length outliers.

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	206	ILE	CA-C-N	7.62	130.82	120.38
1	A	206	ILE	C-N-CA	7.62	130.82	120.38
1	A	180	ASP	CA-C-N	7.06	127.97	119.99
1	A	180	ASP	C-N-CA	7.06	127.97	119.99
1	A	348	THR	CB-CA-C	6.76	117.23	110.33
1	A	184	CYS	CA-C-N	6.58	129.00	120.44
1	A	184	CYS	C-N-CA	6.58	129.00	120.44
1	A	317	ASP	CA-CB-CG	6.57	119.17	112.60
1	B	317	ASP	CA-CB-CG	6.56	119.16	112.60
1	B	348	THR	CB-CA-C	6.22	116.67	110.33
1	B	211	ASN	CA-CB-CG	6.18	118.78	112.60
1	B	488	PHE	CA-CB-CG	6.15	119.95	113.80
1	A	488	PHE	CA-CB-CG	6.05	119.85	113.80
1	A	435	ASN	CA-CB-CG	6.01	118.61	112.60
1	A	543	LYS	CA-C-N	5.89	128.09	120.44
1	A	543	LYS	C-N-CA	5.89	128.09	120.44
1	A	211	ASN	CA-CB-CG	5.85	118.45	112.60
1	B	543	LYS	CA-C-N	5.76	127.93	120.44
1	B	543	LYS	C-N-CA	5.76	127.93	120.44
1	A	450	ASN	CA-CB-CG	5.56	118.16	112.60
1	B	450	ASN	CA-CB-CG	5.49	118.09	112.60
1	B	435	ASN	CA-CB-CG	5.36	117.96	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	489	ILE	CA-C-N	5.34	128.21	120.79
1	B	489	ILE	C-N-CA	5.34	128.21	120.79
1	A	535	GLY	CA-C-N	5.33	128.16	120.38
1	A	535	GLY	C-N-CA	5.33	128.16	120.38
1	B	535	GLY	CA-C-N	5.31	128.13	120.38
1	B	535	GLY	C-N-CA	5.31	128.13	120.38
1	B	371	ILE	CA-C-N	5.26	127.33	120.28
1	B	371	ILE	C-N-CA	5.26	127.33	120.28
1	B	323	ASP	CA-C-N	5.25	127.74	120.29
1	B	323	ASP	C-N-CA	5.25	127.74	120.29
1	B	374	LEU	CA-C-N	5.23	127.71	120.29
1	B	374	LEU	C-N-CA	5.23	127.71	120.29
1	A	469	PHE	CA-CB-CG	5.18	118.98	113.80
1	B	469	PHE	CA-CB-CG	5.17	118.97	113.80
1	A	371	ILE	CA-C-N	5.15	127.18	120.28
1	A	371	ILE	C-N-CA	5.15	127.18	120.28
1	B	475	GLY	CA-C-N	5.09	128.68	121.66
1	B	475	GLY	C-N-CA	5.09	128.68	121.66
1	B	414	PHE	CA-C-N	5.07	127.03	120.44
1	B	414	PHE	C-N-CA	5.07	127.03	120.44
1	A	323	ASP	CA-C-N	5.06	127.48	120.29
1	A	323	ASP	C-N-CA	5.06	127.48	120.29
1	A	300	ASP	CA-CB-CG	5.03	117.63	112.60

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	2902	0	2957	26	0
1	B	2902	0	2957	23	0
2	A	31	0	19	0	0
2	B	31	0	19	0	0
3	A	11	0	3	1	0
3	B	11	0	3	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	24	0	17	0	0
4	B	24	0	17	1	0
5	A	192	0	0	0	0
5	B	177	0	0	2	0
All	All	6305	0	5992	49	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 4.

All (49) 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:281:MET:HE3	1:A:285:LYS:HG2	1.71	0.72
1:B:281:MET:HE3	1:B:285:LYS:HG2	1.71	0.72
1:A:238:LEU:HD13	1:A:306:HIS:HB3	1.79	0.65
1:A:450:ASN:HB2	1:B:254:GLY:O	1.96	0.64
1:A:460:THR:HG21	1:A:463:ILE:HD12	1.79	0.63
1:B:238:LEU:HD13	1:B:306:HIS:HB3	1.80	0.63
1:B:436:GLN:O	1:B:440:LYS:HG3	2.01	0.61
1:B:466:ILE:HD11	1:B:480:LYS:HG3	1.83	0.61
1:A:470:GLU:HG3	1:A:471:ASN:H	1.66	0.60
1:B:470:GLU:HG3	1:B:471:ASN:H	1.67	0.59
1:A:459:THR:HG22	1:A:477:SER:HB3	1.88	0.56
1:B:460:THR:HG21	1:B:463:ILE:HD12	1.89	0.55
1:B:549:LEU:HD13	5:B:2152:HOH:O	2.06	0.55
1:A:210:THR:HB	1:A:558:LEU:HD22	1.91	0.53
1:A:341:ILE:HB	1:A:428:VAL:HG23	1.91	0.53
1:B:341:ILE:HB	1:B:428:VAL:HG23	1.90	0.53
1:B:210:THR:HB	1:B:558:LEU:HD22	1.91	0.52
1:B:539:ALA:HA	1:B:542:ILE:HG22	1.92	0.52
1:A:539:ALA:HA	1:A:542:ILE:HG22	1.92	0.51
1:A:215:LEU:HD22	1:A:425:LEU:HD12	1.93	0.50
1:B:215:LEU:HD22	1:B:425:LEU:HD12	1.94	0.50
1:B:192:GLY:HA3	1:B:233:CYS:SG	2.52	0.49
1:B:337:ASP:OD1	1:B:418:ASN:HB2	2.13	0.49
1:A:192:GLY:HA3	1:A:233:CYS:SG	2.54	0.48
1:A:337:ASP:OD1	1:A:418:ASN:HB2	2.13	0.47
1:A:176:LEU:HD23	1:A:265:ARG:HE	1.80	0.47
1:A:276:CYS:HB2	3:A:900:ORO:O71	2.14	0.46
1:B:185:HIS:HE1	1:B:227:PHE:O	1.98	0.46
1:A:429:LYS:HG3	1:A:455:ILE:HB	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:466:ILE:HD11	1:A:480:LYS:HG3	1.97	0.45
1:B:276:CYS:HB2	3:B:900:ORO:O71	2.17	0.45
1:B:460:THR:CG2	1:B:463:ILE:HD12	2.47	0.44
1:A:539:ALA:O	1:A:543:LYS:HG3	2.18	0.44
1:A:206:ILE:O	1:A:209:CYS:HB2	2.18	0.43
4:B:4000:XBL:H18	4:B:4000:XBL:H82C	2.00	0.43
1:A:456:ILE:HA	1:A:457:SER:HA	1.78	0.42
1:A:503:ILE:HG23	1:A:524:VAL:HG23	2.01	0.42
1:B:206:ILE:HA	1:B:209:CYS:SG	2.59	0.42
1:A:244:PHE:HE2	1:A:526:GLN:HE21	1.67	0.42
1:A:345:SER:H	1:A:351:LEU:HD23	1.84	0.42
1:A:244:PHE:HA	1:A:307:ILE:O	2.20	0.42
1:B:459:THR:HG22	1:B:477:SER:OG	2.21	0.41
1:A:262:ARG:HH12	1:A:279:ASN:HB3	1.86	0.41
1:B:539:ALA:O	1:B:543:LYS:HG3	2.20	0.41
1:A:281:MET:HE1	1:A:289:ASN:HD21	1.86	0.41
1:B:309:GLY:HA3	1:B:338:TYR:CZ	2.56	0.41
1:B:229:LYS:HD2	5:B:2015:HOH:O	2.19	0.40
1:B:281:MET:HE1	1:B:289:ASN:HD21	1.87	0.40
1:A:309:GLY:HA3	1:A:338:TYR:CZ	2.57	0.40

There are no symmetry-related clashes.

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	363/401 (90%)	339 (93%)	22 (6%)	2 (1%)	21	42
1	B	363/401 (90%)	338 (93%)	23 (6%)	2 (1%)	21	42
All	All	726/802 (90%)	677 (93%)	45 (6%)	4 (1%)	21	42

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	204	ASP
1	A	470	GLU
1	B	204	ASP
1	B	470	GLU

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	324/354 (92%)	309 (95%)	15 (5%)	24	50
1	B	324/354 (92%)	310 (96%)	14 (4%)	26	52
All	All	648/708 (92%)	619 (96%)	29 (4%)	24	50

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	167	LEU
1	A	172	LEU
1	A	177	LYS
1	A	187	LEU
1	A	202	SER
1	A	203	ASN
1	A	205	SER
1	A	215	LEU
1	A	265	ARG
1	A	307	ILE
1	A	320	ASN
1	A	331	LYS
1	A	347	ASN
1	A	426	VAL
1	A	484	ILE
1	B	167	LEU
1	B	172	LEU
1	B	177	LYS
1	B	202	SER
1	B	203	ASN

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Mol	Chain	Res	Type
1	B	215	LEU
1	B	265	ARG
1	B	320	ASN
1	B	347	ASN
1	B	426	VAL
1	B	477	SER
1	B	484	ILE
1	B	485	SER
1	B	524	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	185	HIS
1	A	330	ASN
1	A	373	ASN
1	A	377	ASN
1	A	464	ASN
1	A	494	ASN
1	A	526	GLN
1	A	541	GLN
1	A	552	GLN
1	B	330	ASN
1	B	354	ASN
1	B	373	ASN
1	B	436	GLN
1	B	450	ASN
1	B	464	ASN
1	B	526	GLN
1	B	541	GLN
1	B	552	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$
4	XBL	A	4000	-	28,28,28	0.36	0	37,41,41	1.04	2 (5%)
3	ORO	A	900	-	11,11,11	0.26	0	14,15,15	0.37	0
2	FMN	B	800	-	33,33,33	0.51	0	48,50,50	0.49	0
3	ORO	B	900	-	11,11,11	0.26	0	14,15,15	0.33	0
2	FMN	A	800	-	33,33,33	0.44	0	48,50,50	0.51	0
4	XBL	B	4000	-	28,28,28	0.38	0	37,41,41	1.00	2 (5%)

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
4	XBL	A	4000	-	-	2/4/13/13	0/5/5/5
3	ORO	A	900	-	-	2/4/4/4	0/1/1/1
2	FMN	B	800	-	-	1/18/18/18	0/3/3/3
3	ORO	B	900	-	-	2/4/4/4	0/1/1/1
2	FMN	A	800	-	-	1/18/18/18	0/3/3/3
4	XBL	B	4000	-	-	0/4/13/13	0/5/5/5

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	4000	XBL	C14-C2-N2	-4.89	115.06	118.37

Continued on next page...

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	4000	XBL	C14-C2-N2	-4.83	115.10	118.37
4	A	4000	XBL	N4-C3-N3	-2.45	113.54	117.75
4	B	4000	XBL	N4-C3-N3	-2.31	113.78	117.75

There are no chirality outliers.

All (8) torsion outliers are listed below:

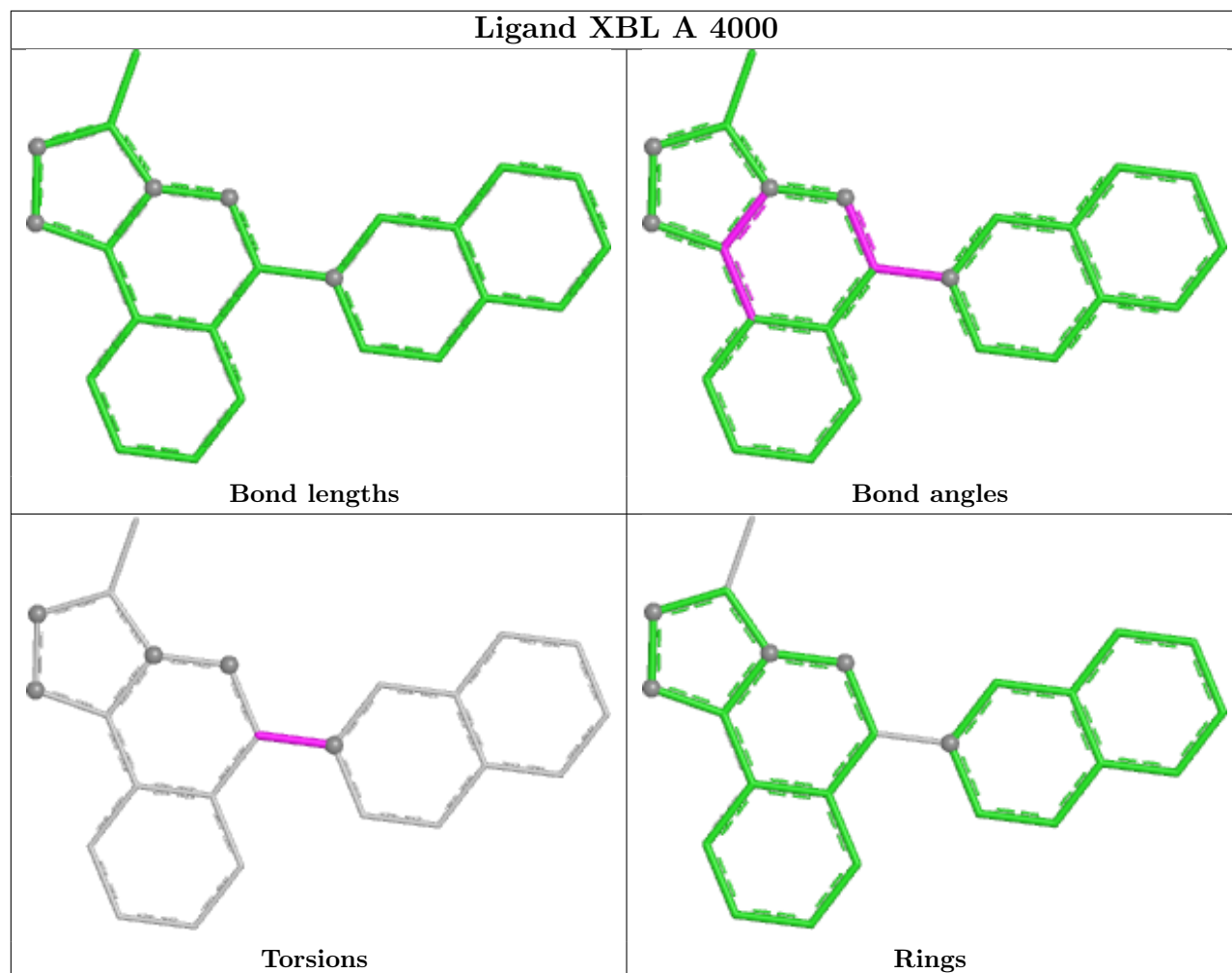
Mol	Chain	Res	Type	Atoms
3	A	900	ORO	N1-C6-C7-O71
3	A	900	ORO	N1-C6-C7-O72
3	B	900	ORO	N1-C6-C7-O71
3	B	900	ORO	N1-C6-C7-O72
4	A	4000	XBL	N3-C3-N4-C8
4	A	4000	XBL	N3-C3-N4-C4
2	A	800	FMN	C4'-C5'-O5'-P
2	B	800	FMN	C4'-C5'-O5'-P

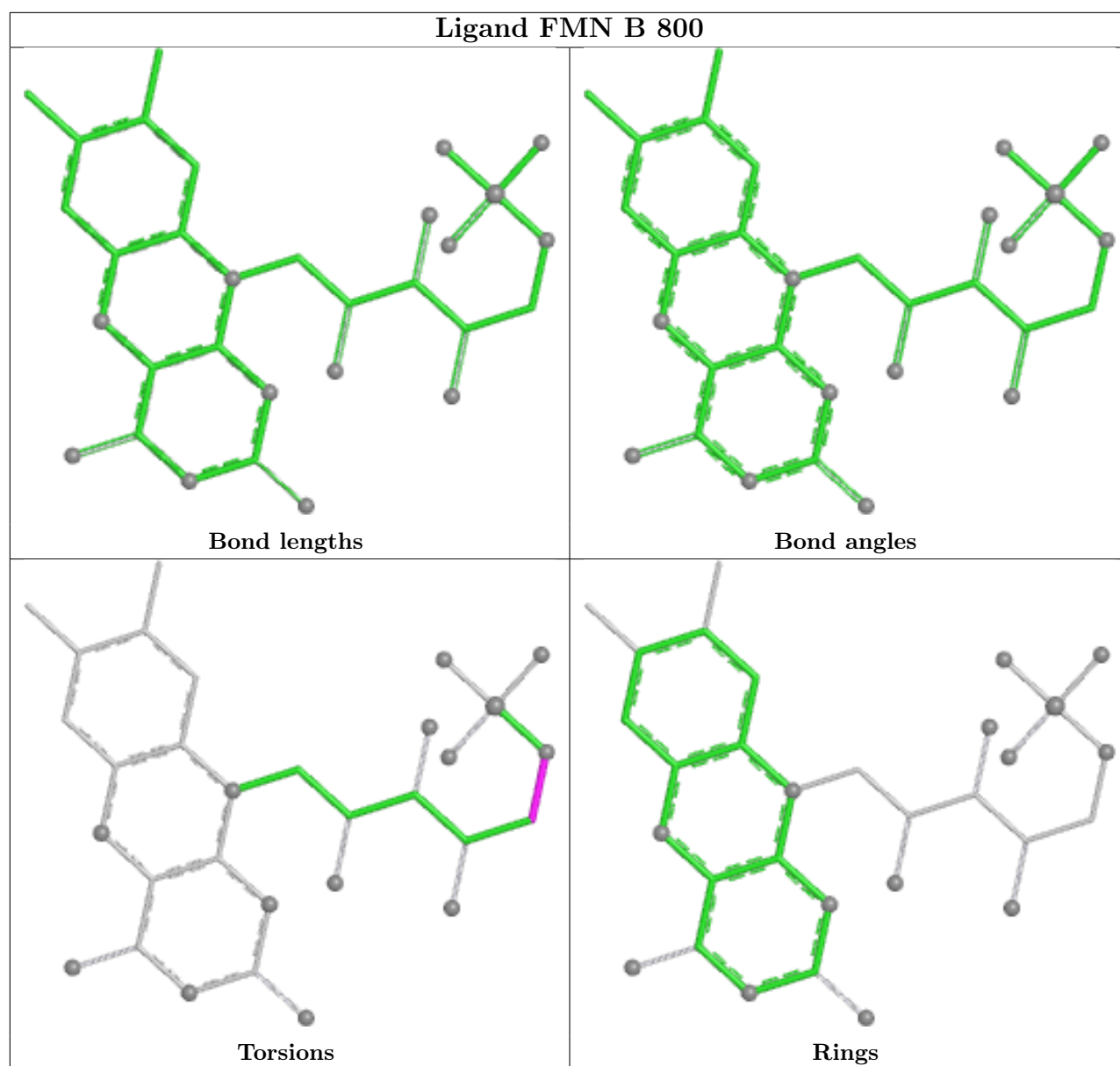
There are no ring outliers.

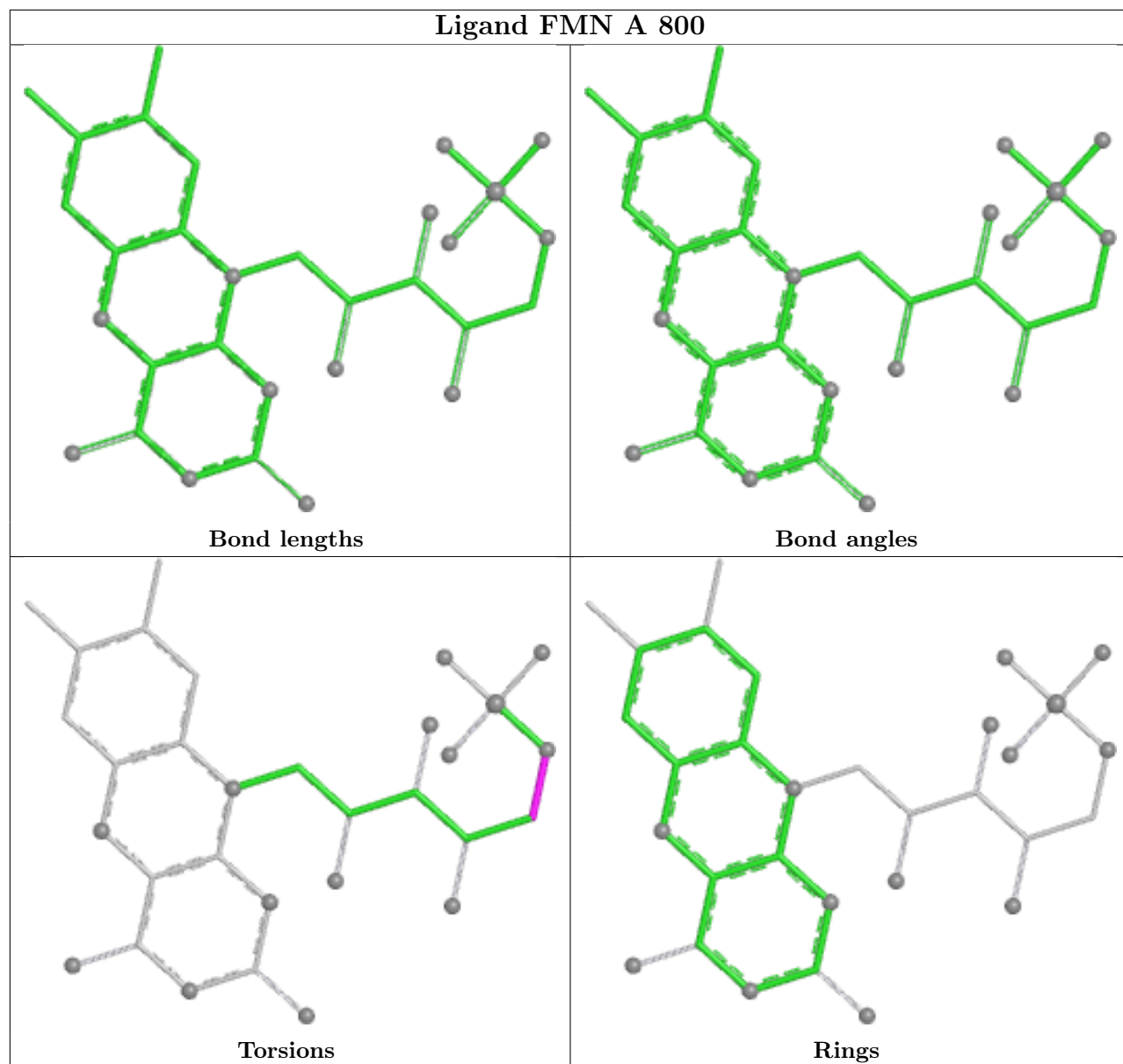
3 monomers are involved in 3 short contacts:

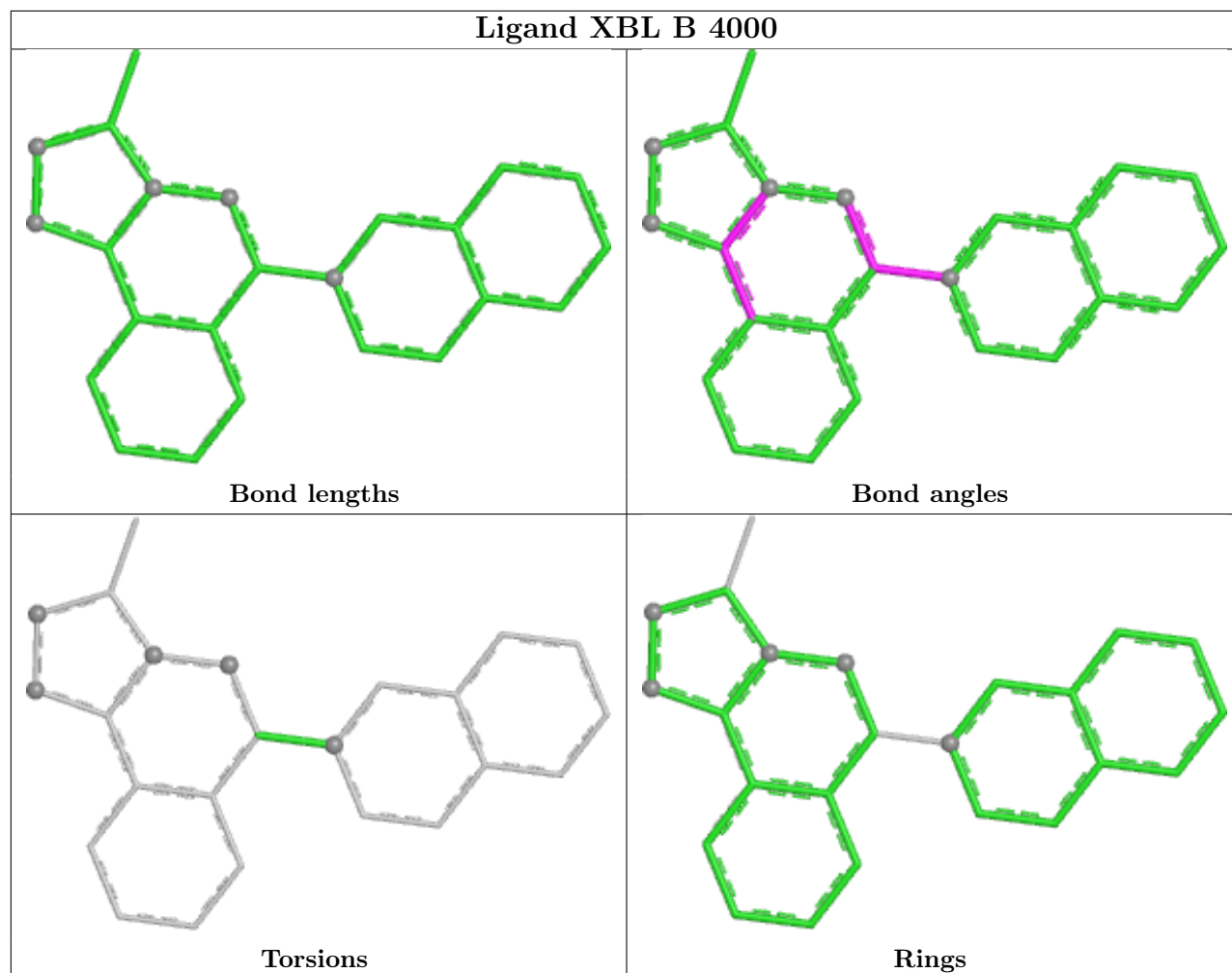
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	900	ORO	1	0
3	B	900	ORO	1	0
4	B	4000	XBL	1	0

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	367/401 (91%)	-1.60	0 100 100	33, 59, 93, 118	0
1	B	367/401 (91%)	-1.59	0 100 100	35, 58, 96, 126	0
All	All	734/802 (91%)	-1.59	0 100 100	33, 58, 95, 126	0

There are no RSRZ outliers to report.

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](#)

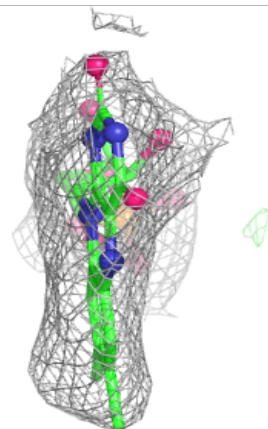
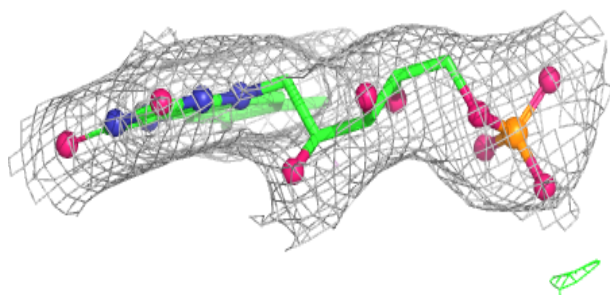
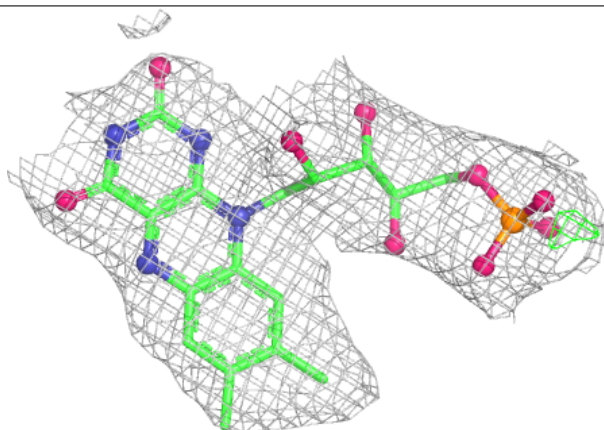
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	FMN	A	800	31/31	1.00	0.02	40,48,53,58	0
2	FMN	B	800	31/31	1.00	0.02	25,47,62,64	0
3	ORO	A	900	11/11	1.00	0.02	29,43,45,48	0
3	ORO	B	900	11/11	1.00	0.01	56,57,59,60	0
4	XBL	A	4000	24/24	1.00	0.03	45,54,61,64	0
4	XBL	B	4000	24/24	1.00	0.03	42,53,59,61	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.

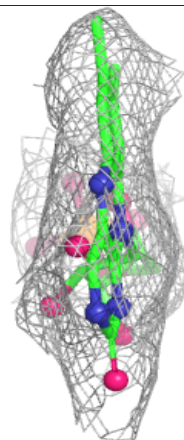
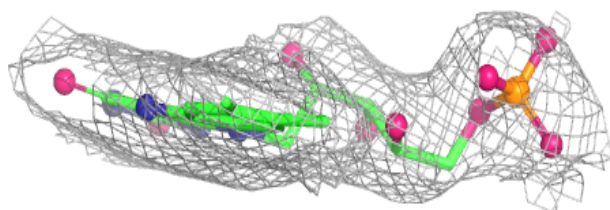
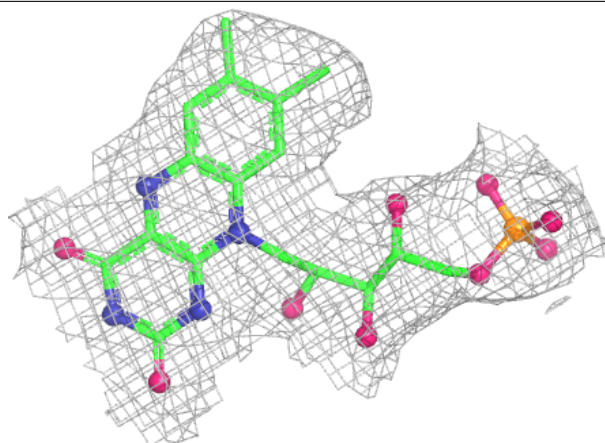
Electron density around FMN A 800:

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

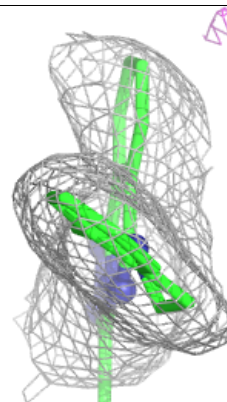
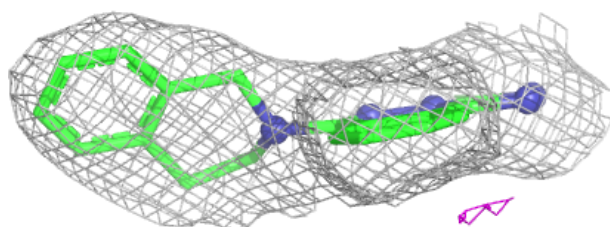
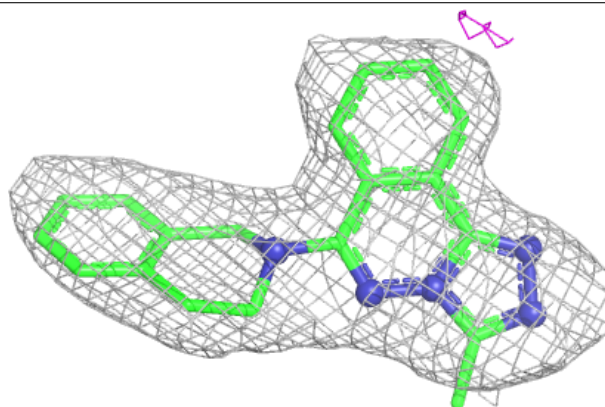


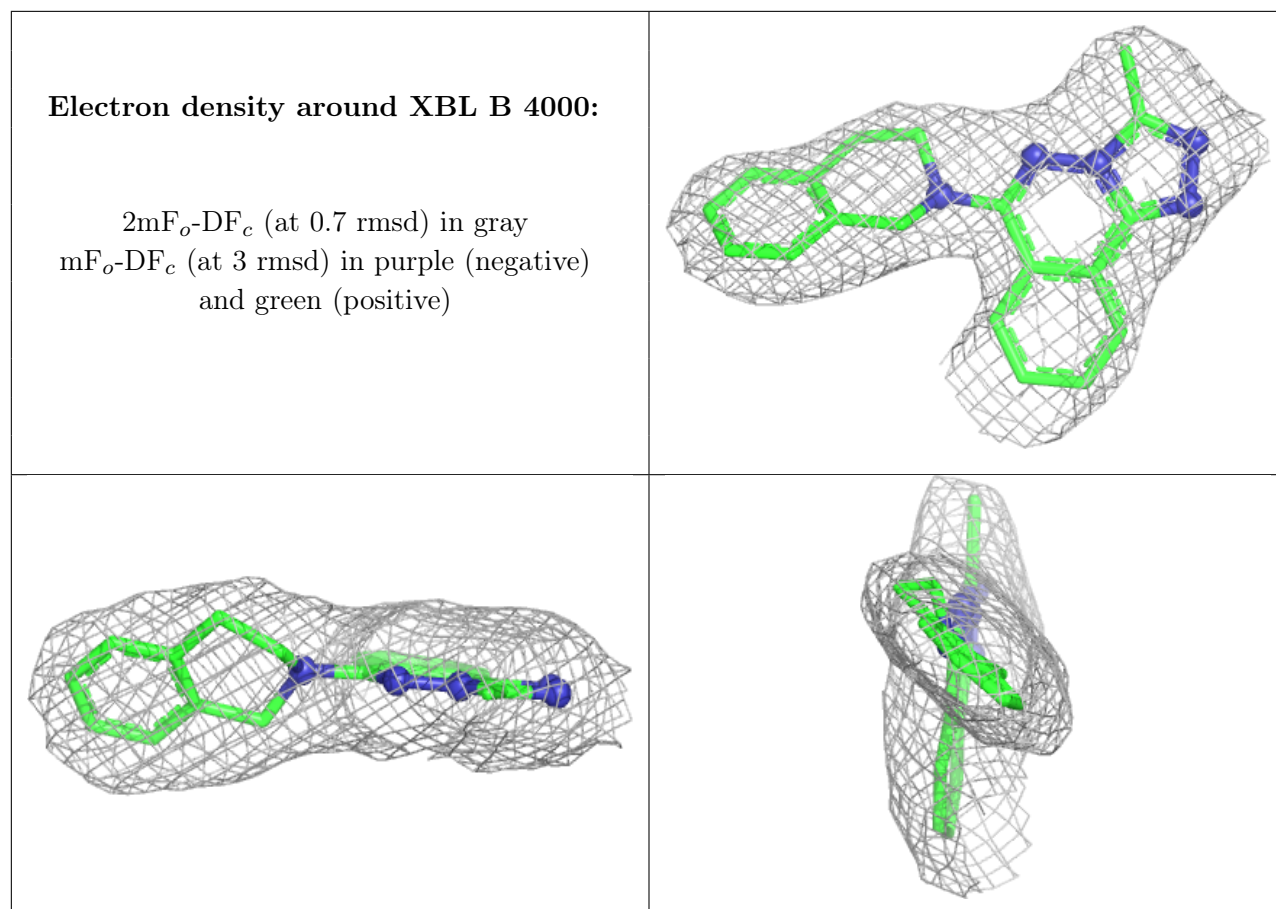
Electron density around FMN B 800:

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

**Electron density around XBL A 4000:**

$2mF_o-DF_c$ (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.