



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 10, 2022 – 08:43 PM EST

PDB ID : 2B4G
Title : dihydroorotate dehydrogenase
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Deposited on : 2005-09-23
Resolution : 1.95 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.31.2
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)	:	2.31.2

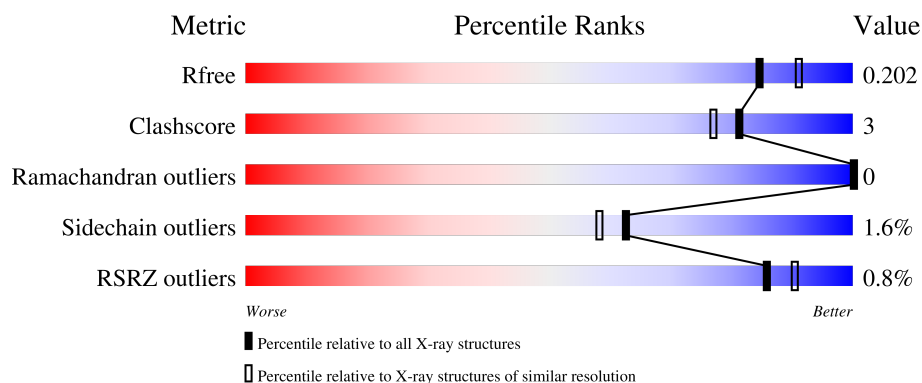
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

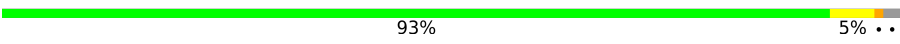



The reported resolution of this entry is 1.95 Å.

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}	130704	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

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	317	 93% 5% ..
1	B	317	 92% 6% .
1	C	317	 92% 6% .
1	D	317	 90% 8% ..

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
2	BR	A	1411	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 10487 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	312	Total	C	N	O	S	0	4	0
			2415	1548	397	454	16			
1	B	313	Total	C	N	O	S	0	4	0
			2422	1553	402	450	17			
1	C	313	Total	C	N	O	S	0	3	0
			2416	1547	400	452	17			
1	D	312	Total	C	N	O	S	0	1	0
			2393	1534	396	447	16			

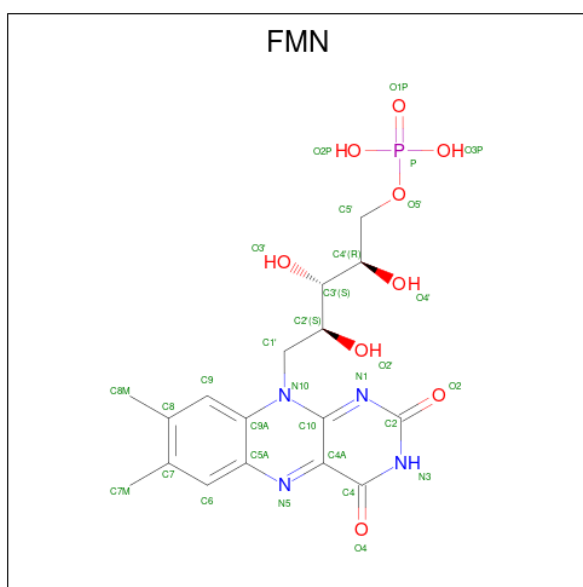
There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	expression tag	UNP Q57U83
A	-2	PRO	-	expression tag	UNP Q57U83
A	-1	GLY	-	expression tag	UNP Q57U83
A	0	SER	-	expression tag	UNP Q57U83
A	115	VAL	ALA	see remark 999	UNP Q57U83
B	-3	GLY	-	expression tag	UNP Q57U83
B	-2	PRO	-	expression tag	UNP Q57U83
B	-1	GLY	-	expression tag	UNP Q57U83
B	0	SER	-	expression tag	UNP Q57U83
B	115	VAL	ALA	see remark 999	UNP Q57U83
C	-3	GLY	-	expression tag	UNP Q57U83
C	-2	PRO	-	expression tag	UNP Q57U83
C	-1	GLY	-	expression tag	UNP Q57U83
C	0	SER	-	expression tag	UNP Q57U83
C	115	VAL	ALA	see remark 999	UNP Q57U83
D	-3	GLY	-	expression tag	UNP Q57U83
D	-2	PRO	-	expression tag	UNP Q57U83
D	-1	GLY	-	expression tag	UNP Q57U83
D	0	SER	-	expression tag	UNP Q57U83
D	115	VAL	ALA	see remark 999	UNP Q57U83

- Molecule 2 is BROMIDE ION (three-letter code: BR) (formula: Br).

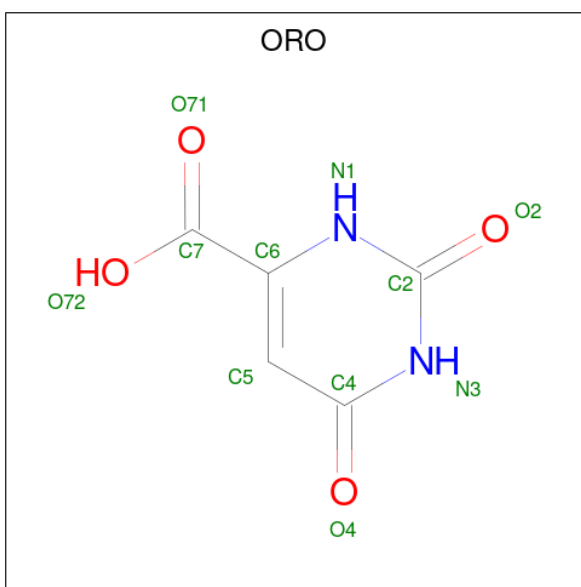
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	4	Total	Br	0	0
			4	4		
2	B	2	Total	Br	0	0
			2	2		
2	C	3	Total	Br	0	0
			3	3		
2	D	2	Total	Br	0	0
			2	2		

- Molecule 3 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: C₁₇H₂₁N₄O₉P).



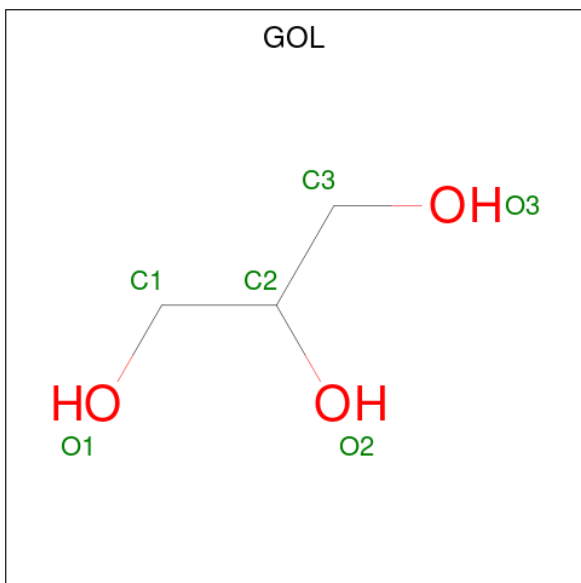
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
3	B	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
3	C	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
3	D	1	Total	C	N	O	P	0	0
			31	17	4	9	1		

- Molecule 4 is OROTIC ACID (three-letter code: ORO) (formula: C₅H₄N₂O₄).



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

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	C	1	Total	C	O	0	0
			6	3	3		
5	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	180	Total	O	0	0
			180	180		
6	B	143	Total	O	0	0
			143	143		
6	C	159	Total	O	0	0
			159	159		
6	D	156	Total	O	0	0
			156	156		

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

Chain A:  93% 5% ..

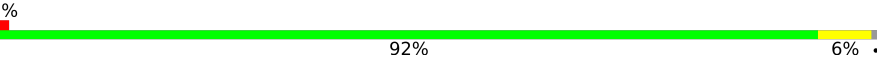


- Molecule 1: dihydroorotate dehydrogenase

Chain B:  92% 6% ..




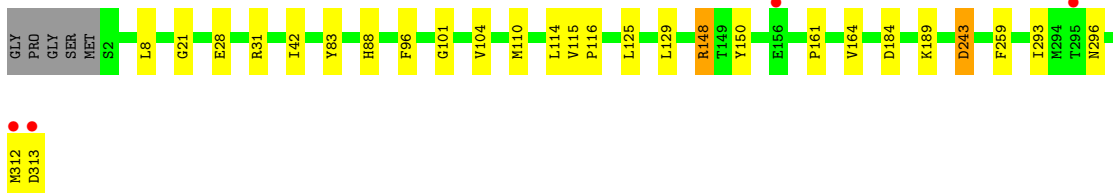
- Molecule 1: dihydroorotate dehydrogenase

Chain C:  92% 6% ..



- Molecule 1: dihydroorotate dehydrogenase

Chain D:  90% 8% ..



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	81.61Å 162.63Å 163.07Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 1.95 20.88 – 1.95	Depositor EDS
% Data completeness (in resolution range)	96.0 (50.00-1.95) 96.1 (20.88-1.95)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.84 (at 1.95Å)	Xtriage
Refinement program	REFMAC refmac_ 5.2.0005 24/04/2001	Depositor
R, R_{free}	0.189 , 0.242 0.202 , 0.202	Depositor DCC
R_{free} test set	3825 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	15.4	Xtriage
Anisotropy	0.421	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 44.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.53$, $\langle L^2 \rangle = 0.37$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	10487	wwPDB-VP
Average B, all atoms (Å ²)	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 51.69 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 5.4125e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: BR, ORO, GOL, FMN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.55	0/2483	0.65	1/3361 (0.0%)
1	B	0.55	0/2488	0.64	1/3366 (0.0%)
1	C	0.55	0/2478	0.66	0/3352
1	D	0.55	0/2449	0.66	2/3315 (0.1%)
All	All	0.55	0/9898	0.65	4/13394 (0.0%)

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	D	0	1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	306	ARG	NE-CZ-NH1	6.37	123.48	120.30
1	D	148	ARG	NE-CZ-NH1	5.95	123.27	120.30
1	D	148	ARG	NE-CZ-NH2	-5.38	117.61	120.30
1	A	148	ARG	NE-CZ-NH1	5.07	122.83	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	312	MET	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	2415	0	2428	11	0
1	B	2422	0	2444	12	0
1	C	2416	0	2432	11	0
1	D	2393	0	2406	18	0
2	A	4	0	0	2	0
2	B	2	0	0	0	0
2	C	3	0	0	0	0
2	D	2	0	0	1	0
3	A	31	0	19	1	0
3	B	31	0	19	1	0
3	C	31	0	19	1	0
3	D	31	0	19	1	0
4	A	11	0	3	0	0
4	B	11	0	3	0	0
4	C	11	0	3	0	0
4	D	11	0	3	0	0
5	A	12	0	16	0	0
5	C	6	0	8	0	1
5	D	6	0	8	0	0
6	A	180	0	0	0	1
6	B	143	0	0	2	0
6	C	159	0	0	2	0
6	D	156	0	0	3	0
All	All	10487	0	9830	51	1

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 3.

All (51) 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:28[B]:GLU:OE2	1:B:31[B]:ARG:NH2	1.71	1.22
1:B:28[B]:GLU:CD	1:B:31[B]:ARG:HH21	1.81	0.83
1:D:296:ASN:ND2	6:D:4552:HOH:O	2.14	0.81
1:B:137:LYS:O	6:B:2549:HOH:O	2.02	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:301:THR:OG1	1:C:303[A]:ASP:OD1	2.05	0.72
1:B:28[B]:GLU:OE1	1:B:31[B]:ARG:NE	2.26	0.66
1:B:266:ALA:O	1:B:306:ARG:HD3	1.96	0.65
1:A:139:GLN:OE1	2:A:1411:BR:BR	2.70	0.65
1:D:148:ARG:NH2	1:D:184:ASP:OD2	2.33	0.62
1:D:243:ASP:HB2	6:D:4559:HOH:O	2.02	0.60
1:D:259:PHE:HB2	1:D:293:ILE:HD11	1.86	0.57
1:C:21:GLY:HA3	3:C:3400:FMN:N5	2.20	0.57
1:A:148:ARG:NH2	1:A:184:ASP:OD2	2.38	0.56
1:B:45:SER:HB3	1:B:100:SER:OG	2.06	0.56
1:D:21:GLY:HA3	3:D:4400:FMN:N5	2.22	0.55
1:B:21:GLY:HA3	3:B:2400:FMN:N5	2.24	0.52
1:A:28:GLU:OE1	1:C:256:GLU:HG2	2.11	0.50
1:C:92:ARG:HD2	6:C:4564:HOH:O	2.10	0.49
1:D:259:PHE:HB2	1:D:293:ILE:CD1	2.42	0.49
1:C:161:PRO:HB3	1:C:189:LYS:HG3	1.93	0.49
1:D:161:PRO:HB3	1:D:189:LYS:HG3	1.94	0.49
1:D:83:TYR:CE2	1:D:88:HIS:HB2	2.48	0.48
1:D:129:LEU:HD12	1:D:164[B]:VAL:HG11	1.94	0.48
1:C:83:TYR:CE2	1:C:88:HIS:HB2	2.48	0.48
1:B:227:LEU:HB3	1:B:228:PRO:HD3	1.96	0.48
1:A:197:ILE:HD12	1:A:226[A]:VAL:HG12	1.96	0.47
1:C:55:PRO:CB	1:C:213:LYS:HD3	2.44	0.47
1:C:55:PRO:HB2	1:C:213:LYS:HD3	1.97	0.47
1:D:28:GLU:OE1	1:D:31:ARG:NE	2.47	0.47
1:A:4:LYS:HZ2	1:A:4:LYS:CB	2.28	0.47
1:B:28[B]:GLU:CD	1:B:31[B]:ARG:HE	2.15	0.47
1:C:48:LEU:HD12	1:C:106:GLU:HG3	1.96	0.47
1:A:21:GLY:HA3	3:A:1400:FMN:N5	2.30	0.46
1:B:86:GLN:NE2	6:B:2471:HOH:O	2.38	0.46
1:D:115:VAL:HB	1:D:116:PRO:HD3	1.98	0.46
1:D:104:VAL:HG13	1:D:150:TYR:CE1	2.51	0.45
1:A:21:GLY:HA2	1:A:44:LYS:HD2	1.99	0.45
1:D:129:LEU:HD12	1:D:164[B]:VAL:CG1	2.47	0.45
1:A:223:GLY:O	1:A:226[B]:VAL:HG12	2.16	0.44
1:A:227:LEU:HB3	1:A:228:PRO:HD3	2.00	0.44
1:D:42:ILE:HA	1:D:96:PHE:O	2.17	0.44
1:C:158:TYR:CE1	1:C:160:LEU:HB2	2.53	0.44
1:B:1:MET:HG3	1:B:291:GLN:HE21	1.82	0.43
1:D:101:GLY:N	1:D:110:MET:HE1	2.33	0.43
1:D:293:ILE:HG23	6:D:4464:HOH:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:152:GLN:NE2	1:B:156:GLU:OE2	2.51	0.43
1:C:3:LEU:O	1:C:14:ASN:HA	2.19	0.42
1:A:199:ASN:ND2	2:A:1411:BR:BR	3.05	0.42
1:D:8:LEU:HA	2:D:4412:BR:BR	2.75	0.41
6:C:4411:HOH:O	1:D:313:ASP:HB2	2.19	0.41
1:A:83:TYR:CE2	1:A:88:HIS:HB2	2.56	0.40

All (1) 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:C:3401:GOL:O2	6:A:1581:HOH:O[8_455]	1.48	0.72

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	315/317 (99%)	304 (96%)	11 (4%)	0	100	100
1	B	315/317 (99%)	306 (97%)	9 (3%)	0	100	100
1	C	314/317 (99%)	304 (97%)	10 (3%)	0	100	100
1	D	311/317 (98%)	297 (96%)	14 (4%)	0	100	100
All	All	1255/1268 (99%)	1211 (96%)	44 (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	267/265 (101%)	262 (98%)	5 (2%)	57	50
1	B	267/265 (101%)	260 (97%)	7 (3%)	46	36
1	C	266/265 (100%)	262 (98%)	4 (2%)	65	60
1	D	263/265 (99%)	260 (99%)	3 (1%)	73	71
All	All	1063/1060 (100%)	1044 (98%)	19 (2%)	62	53

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LYS
1	A	104	VAL
1	A	256[A]	GLU
1	A	256[B]	GLU
1	A	300	LYS
1	B	52	THR
1	B	104[A]	VAL
1	B	104[B]	VAL
1	B	114	LEU
1	B	184	ASP
1	B	256	GLU
1	B	263	LEU
1	C	92	ARG
1	C	114	LEU
1	C	125	LEU
1	C	313	ASP
1	D	114	LEU
1	D	125	LEU
1	D	243	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	216	GLN
1	B	291	GLN
1	C	216	GLN
1	D	296	ASN

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 ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 23 ligands modelled in this entry, 11 are monoatomic - leaving 12 for Mogul analysis.

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	ORO	D	4399	-	9,11,11	1.19	0	8,15,15	1.83	2 (25%)
5	GOL	C	3401	-	5,5,5	0.37	0	5,5,5	0.28	0
3	FMN	A	1400	-	33,33,33	0.96	2 (6%)	48,50,50	1.26	7 (14%)
4	ORO	A	1399	-	9,11,11	1.12	1 (11%)	8,15,15	2.32	3 (37%)
5	GOL	A	1401	-	5,5,5	0.42	0	5,5,5	0.28	0
3	FMN	C	3400	-	33,33,33	1.07	2 (6%)	48,50,50	1.22	6 (12%)
4	ORO	B	2399	-	9,11,11	1.17	0	8,15,15	2.64	4 (50%)
5	GOL	A	1403	-	5,5,5	0.37	0	5,5,5	0.24	0
3	FMN	B	2400	-	33,33,33	1.09	2 (6%)	48,50,50	1.30	9 (18%)
4	ORO	C	3399	-	9,11,11	1.34	1 (11%)	8,15,15	1.74	1 (12%)
5	GOL	D	4401	-	5,5,5	0.51	0	5,5,5	0.35	0
3	FMN	D	4400	-	33,33,33	1.02	2 (6%)	48,50,50	1.29	8 (16%)

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	ORO	D	4399	-	-	4/4/4/4	0/1/1/1
5	GOL	C	3401	-	-	2/4/4/4	-
3	FMN	A	1400	-	-	5/18/18/18	0/3/3/3
4	ORO	A	1399	-	-	4/4/4/4	0/1/1/1
5	GOL	A	1401	-	-	2/4/4/4	-
3	FMN	C	3400	-	-	1/18/18/18	0/3/3/3
4	ORO	B	2399	-	-	4/4/4/4	0/1/1/1
5	GOL	A	1403	-	-	2/4/4/4	-
3	FMN	B	2400	-	-	2/18/18/18	0/3/3/3
4	ORO	C	3399	-	-	4/4/4/4	0/1/1/1
5	GOL	D	4401	-	-	2/4/4/4	-
3	FMN	D	4400	-	-	1/18/18/18	0/3/3/3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	2400	FMN	C4A-N5	4.43	1.39	1.30
3	C	3400	FMN	C4A-N5	4.14	1.38	1.30
3	D	4400	FMN	C4A-N5	3.97	1.38	1.30
3	A	1400	FMN	C4A-N5	3.50	1.37	1.30
3	C	3400	FMN	C10-N1	2.81	1.39	1.33
3	B	2400	FMN	C10-N1	2.35	1.38	1.33
4	C	3399	ORO	C2-N1	-2.23	1.33	1.38
4	A	1399	ORO	C2-N1	-2.23	1.33	1.38
3	D	4400	FMN	C10-N1	2.17	1.37	1.33
3	A	1400	FMN	C10-N1	2.09	1.37	1.33

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	2399	ORO	C5-C4-N3	-5.14	118.08	124.08
4	A	1399	ORO	C5-C4-N3	-4.82	118.45	124.08
4	C	3399	ORO	C5-C4-N3	-4.48	118.85	124.08
4	B	2399	ORO	C6-C5-C4	4.01	119.32	116.73
4	D	4399	ORO	C5-C4-N3	-3.99	119.42	124.08
4	A	1399	ORO	C6-C5-C4	3.20	118.79	116.73
3	D	4400	FMN	C4A-C10-N10	3.16	121.11	116.48
3	A	1400	FMN	C4A-C10-N10	2.97	120.82	116.48
3	C	3400	FMN	C10-C4A-N5	-2.83	118.84	124.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	4400	FMN	C10-C4A-N5	-2.75	119.02	124.86
3	B	2400	FMN	C10-C4A-N5	-2.68	119.17	124.86
3	B	2400	FMN	C4A-C10-N10	2.67	120.38	116.48
3	D	4400	FMN	C4-N3-C2	-2.57	120.90	125.64
3	A	1400	FMN	C9A-C5A-N5	-2.50	119.72	122.43
3	B	2400	FMN	C9A-C5A-N5	-2.42	119.80	122.43
3	C	3400	FMN	C4A-C10-N10	2.36	119.92	116.48
3	B	2400	FMN	C4-N3-C2	-2.34	121.32	125.64
4	A	1399	ORO	C5-C6-N1	-2.33	119.18	123.40
3	A	1400	FMN	C10-C4A-N5	-2.31	119.96	124.86
3	D	4400	FMN	O4-C4-C4A	-2.30	120.50	126.60
3	C	3400	FMN	C7M-C7-C6	-2.27	115.29	119.49
3	A	1400	FMN	C5A-C9A-N10	2.24	120.26	117.95
3	B	2400	FMN	C4-C4A-N5	2.21	121.37	118.23
3	A	1400	FMN	C8M-C8-C9	-2.21	115.41	119.49
3	D	4400	FMN	C4-C4A-N5	2.20	121.36	118.23
3	B	2400	FMN	O4-C4-C4A	-2.19	120.78	126.60
4	B	2399	ORO	O71-C7-C6	2.18	125.67	121.24
3	D	4400	FMN	C8M-C8-C9	-2.17	115.47	119.49
3	C	3400	FMN	C4-C4A-N5	2.17	121.32	118.23
3	D	4400	FMN	O2-C2-N1	-2.14	118.28	121.83
3	A	1400	FMN	C4-C4A-N5	2.13	121.27	118.23
3	C	3400	FMN	C4A-C4-N3	2.12	118.57	113.19
3	D	4400	FMN	C4A-C4-N3	2.09	118.49	113.19
4	D	4399	ORO	C5-C6-N1	-2.08	119.62	123.40
4	B	2399	ORO	C5-C6-N1	-2.08	119.64	123.40
3	B	2400	FMN	C5A-C9A-N10	2.07	120.09	117.95
3	C	3400	FMN	C4-N3-C2	-2.06	121.83	125.64
3	A	1400	FMN	C4A-C4-N3	2.04	118.36	113.19
3	B	2400	FMN	C4A-C4-N3	2.01	118.29	113.19
3	B	2400	FMN	C8M-C8-C9	-2.01	115.78	119.49

There are no chirality outliers.

All (33) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1399	ORO	N1-C6-C7-O71
4	A	1399	ORO	N1-C6-C7-O72
4	A	1399	ORO	C5-C6-C7-O71
4	A	1399	ORO	C5-C6-C7-O72
4	B	2399	ORO	N1-C6-C7-O71
4	B	2399	ORO	N1-C6-C7-O72

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Mol	Chain	Res	Type	Atoms
4	B	2399	ORO	C5-C6-C7-O71
4	B	2399	ORO	C5-C6-C7-O72
4	C	3399	ORO	N1-C6-C7-O71
4	C	3399	ORO	N1-C6-C7-O72
4	C	3399	ORO	C5-C6-C7-O71
4	C	3399	ORO	C5-C6-C7-O72
4	D	4399	ORO	N1-C6-C7-O71
4	D	4399	ORO	N1-C6-C7-O72
4	D	4399	ORO	C5-C6-C7-O71
4	D	4399	ORO	C5-C6-C7-O72
5	A	1401	GOL	C1-C2-C3-O3
5	D	4401	GOL	C1-C2-C3-O3
5	A	1403	GOL	O1-C1-C2-C3
3	A	1400	FMN	C2'-C3'-C4'-O4'
5	A	1401	GOL	O2-C2-C3-O3
5	C	3401	GOL	O2-C2-C3-O3
3	A	1400	FMN	C4'-C5'-O5'-P
3	B	2400	FMN	C4'-C5'-O5'-P
3	C	3400	FMN	C4'-C5'-O5'-P
3	D	4400	FMN	C4'-C5'-O5'-P
5	D	4401	GOL	O2-C2-C3-O3
5	C	3401	GOL	C1-C2-C3-O3
3	B	2400	FMN	C2'-C3'-C4'-O4'
3	A	1400	FMN	O3'-C3'-C4'-O4'
5	A	1403	GOL	O1-C1-C2-O2
3	A	1400	FMN	C2'-C3'-C4'-C5'
3	A	1400	FMN	O3'-C3'-C4'-C5'

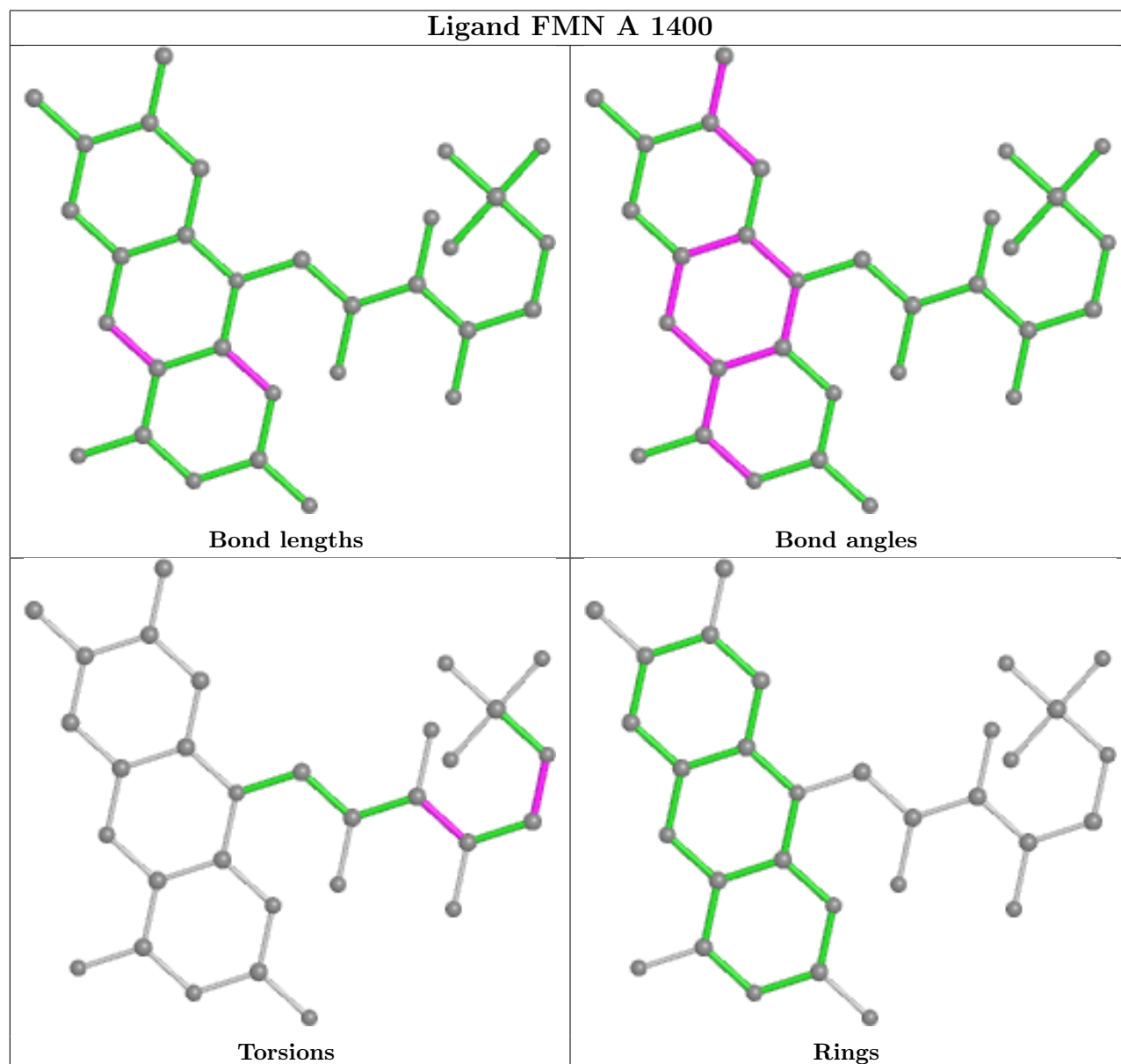
There are no ring outliers.

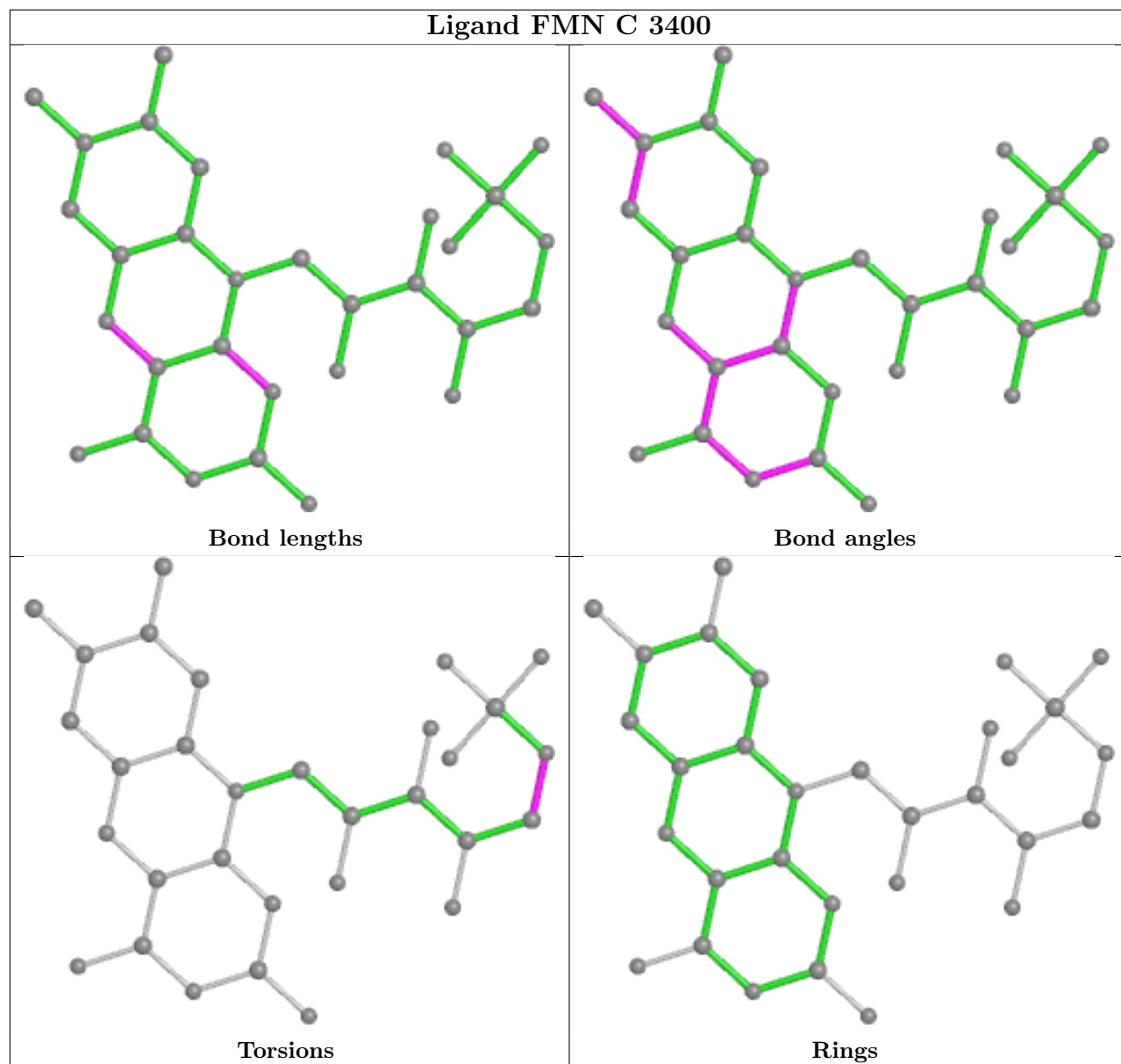
5 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	3401	GOL	0	1
3	A	1400	FMN	1	0
3	C	3400	FMN	1	0
3	B	2400	FMN	1	0
3	D	4400	FMN	1	0

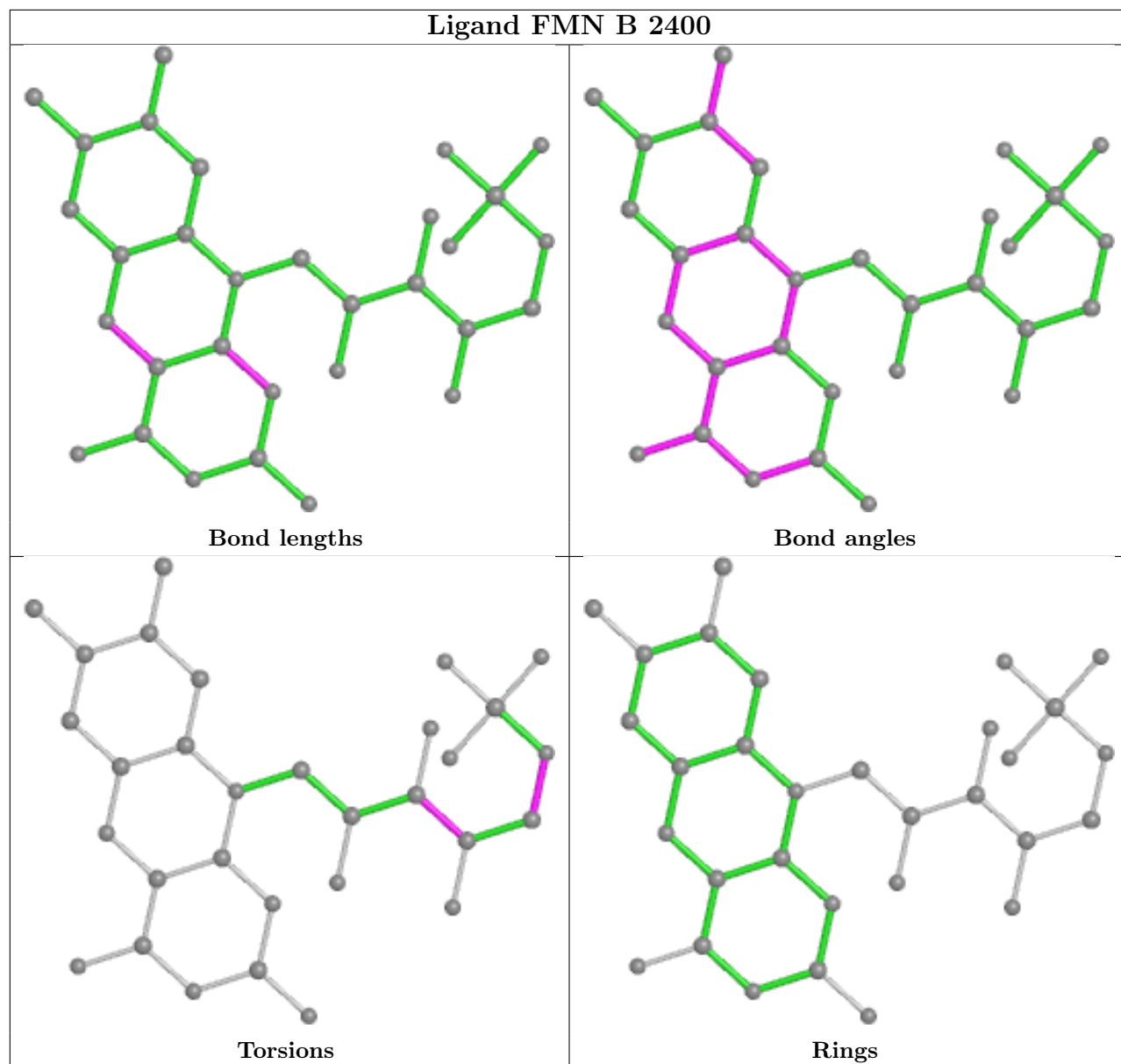
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is

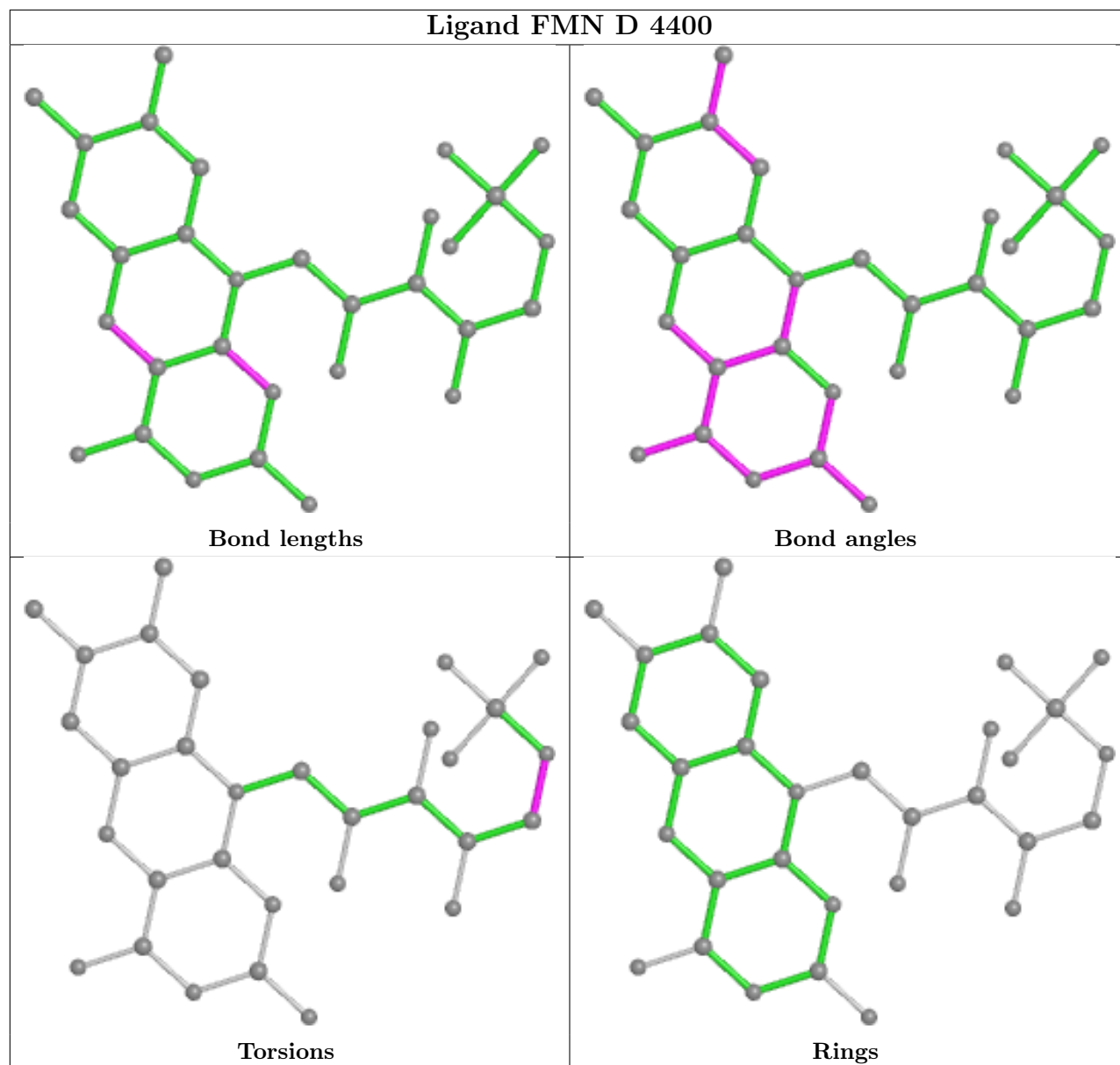
within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question 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.





Ligand FMN B 2400





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	312/317 (98%)	-0.08	1 (0%) 94 96	9, 14, 20, 24	0
1	B	313/317 (98%)	0.04	2 (0%) 89 93	9, 15, 23, 33	0
1	C	313/317 (98%)	-0.01	3 (0%) 82 87	7, 14, 22, 32	0
1	D	312/317 (98%)	0.02	4 (1%) 77 83	8, 15, 22, 34	0
All	All	1250/1268 (98%)	-0.01	10 (0%) 86 90	7, 15, 22, 34	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	313	ASP	5.7
1	B	313	ASP	4.2
1	C	313	ASP	3.7
1	A	243[A]	ASP	3.0
1	D	156	GLU	2.5
1	C	1	MET	2.2
1	D	295	THR	2.2
1	C	11	GLU	2.2
1	B	100	SER	2.1
1	D	312	MET	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 monosaccharides in this entry.

6.4 Ligands ⓘ

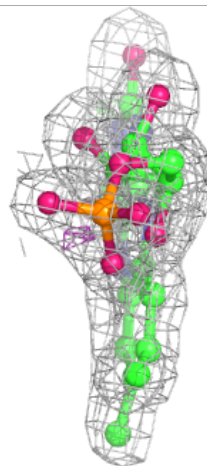
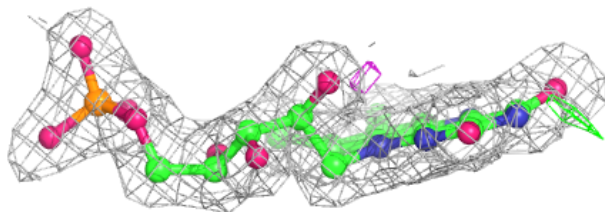
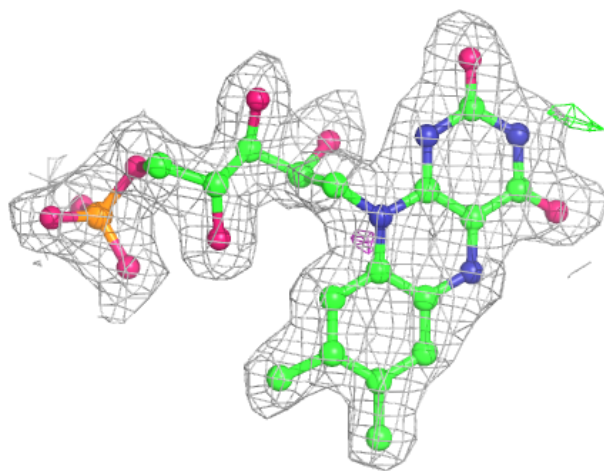
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	GOL	C	3401	6/6	0.70	0.30	55,55,56,56	0
5	GOL	A	1403	6/6	0.75	0.16	40,42,42,43	0
2	BR	C	4410	1/1	0.83	0.15	36,36,36,36	1
2	BR	A	1414	1/1	0.85	0.10	32,32,32,32	1
2	BR	D	4411	1/1	0.90	0.14	30,30,30,30	1
4	ORO	C	3399	11/11	0.93	0.11	11,12,13,14	0
5	GOL	A	1401	6/6	0.93	0.12	23,24,25,25	0
2	BR	A	1415	1/1	0.94	0.18	41,41,41,41	1
2	BR	C	3411	1/1	0.95	0.10	32,32,32,32	1
2	BR	D	4412	1/1	0.95	0.19	32,32,32,32	1
4	ORO	A	1399	11/11	0.95	0.10	9,11,12,12	0
4	ORO	B	2399	11/11	0.95	0.09	10,12,13,13	0
5	GOL	D	4401	6/6	0.95	0.12	25,27,27,28	0
3	FMN	D	4400	31/31	0.96	0.10	8,11,11,13	0
2	BR	B	2410	1/1	0.96	0.06	21,21,21,21	1
3	FMN	B	2400	31/31	0.96	0.10	8,14,16,16	0
3	FMN	C	3400	31/31	0.96	0.09	8,11,13,13	0
3	FMN	A	1400	31/31	0.97	0.09	8,11,12,14	0
4	ORO	D	4399	11/11	0.97	0.08	7,8,10,10	0
2	BR	B	1413	1/1	0.97	0.08	27,27,27,27	1
2	BR	A	1412	1/1	0.99	0.03	28,28,28,28	1
2	BR	C	3410	1/1	0.99	0.03	16,16,16,16	1
2	BR	A	1411	1/1	0.99	0.11	28,28,28,28	1

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.

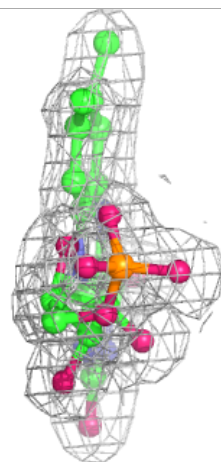
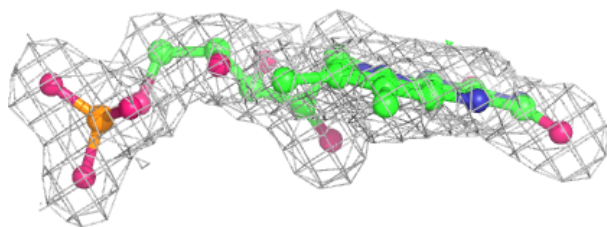
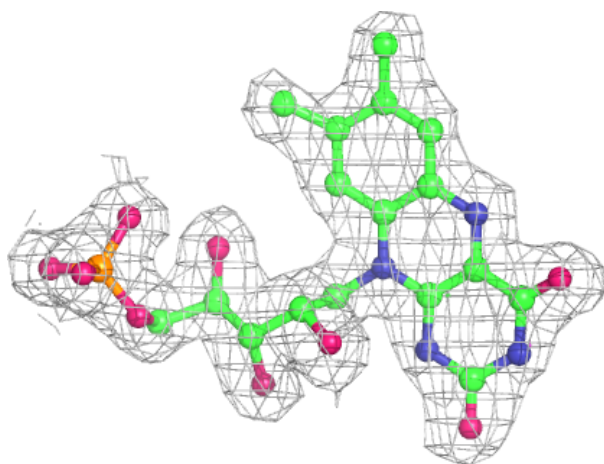
Electron density around FMN D 4400:

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



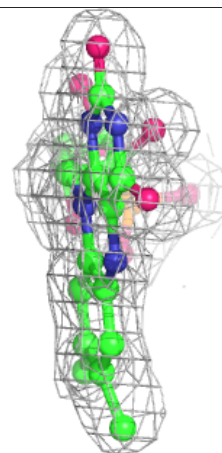
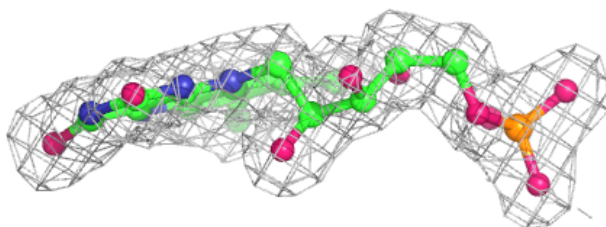
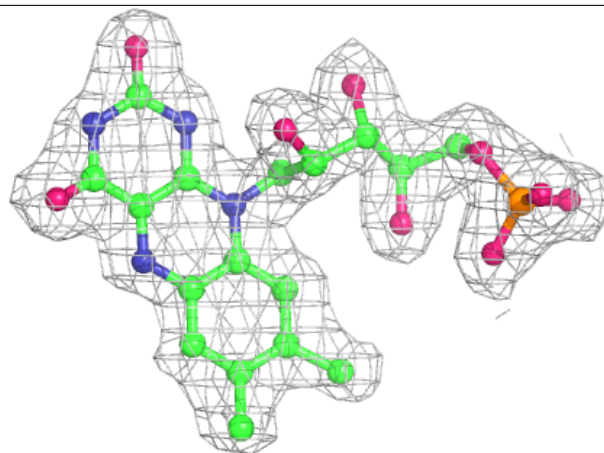
Electron density around FMN B 2400:

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



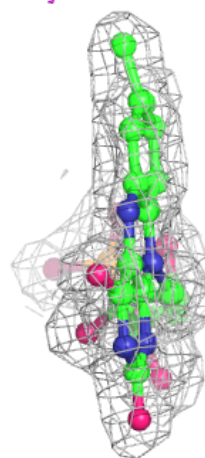
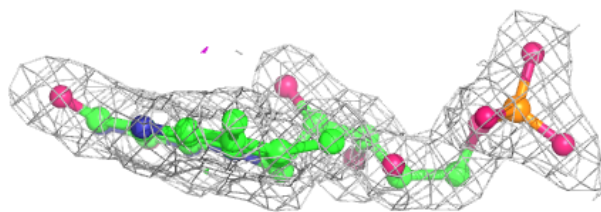
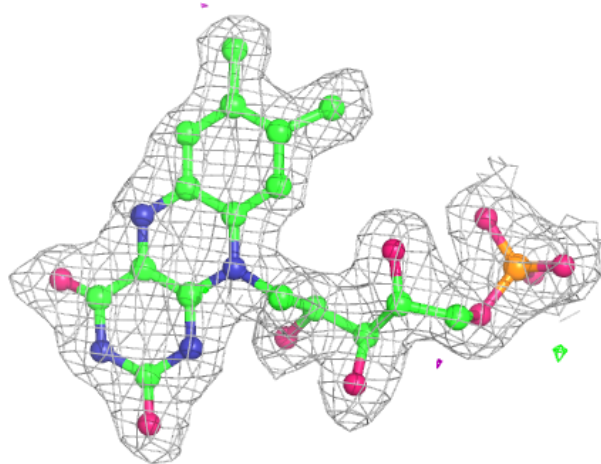
Electron density around FMN C 3400:

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



Electron density around FMN A 1400:

$2mF_o-DF_c$ (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.