



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 26, 2020 – 12:37 PM EDT

PDB ID : 6VND
Title : Quaternary Complex of human dihydroorotate dehydrogenase (DHODH) with
flavin mononucleotide (FMN), orotic acid and AG-636
Authors : Padyana, A.; Jin, L.
Deposited on : 2020-01-29
Resolution : 1.97 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 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 : 2.14.6
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) : 2.14.6

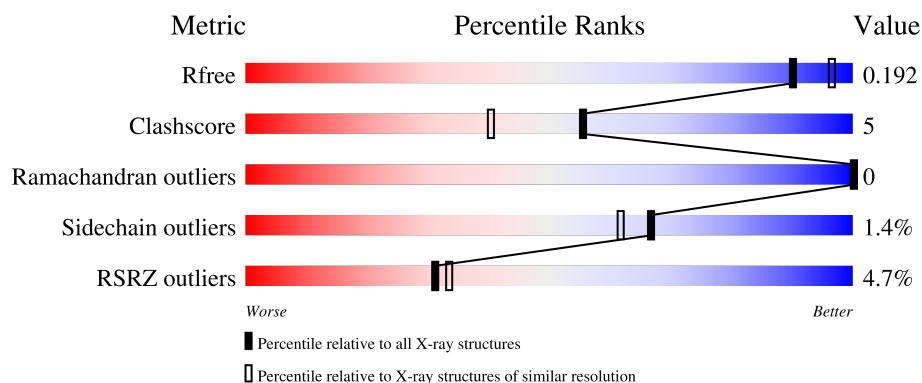
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.97 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	11647 (2.00-1.96)
Clashscore	141614	1014 (1.98-1.98)
Ramachandran outliers	138981	1006 (1.98-1.98)
Sidechain outliers	138945	1006 (1.98-1.98)
RSRZ outliers	127900	11410 (2.00-1.96)

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 on 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	368	<div> <div>5%</div> <div>91%</div> <div>8% ..</div> </div>

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
10	GOL	A	417	-	-	X	-

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.

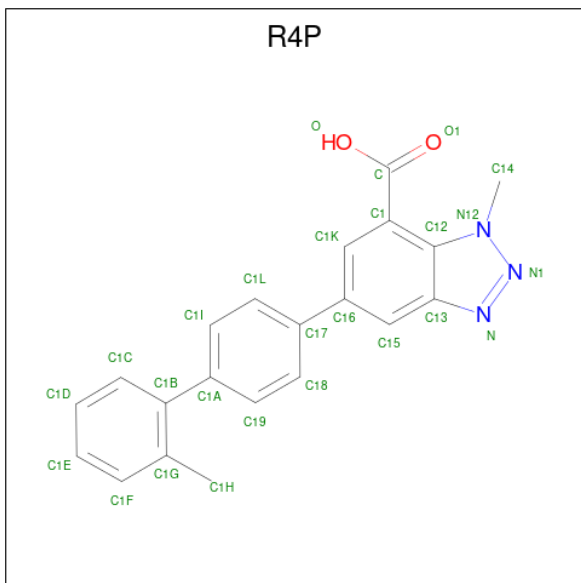
- Molecule 1 is a protein called Dihydroorotate dehydrogenase (quinone), mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	365	Total	C	N	O	S	6	5	0
			2810	1766	517	523	4			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	28	GLY	-	cloning artifact	UNP Q02127

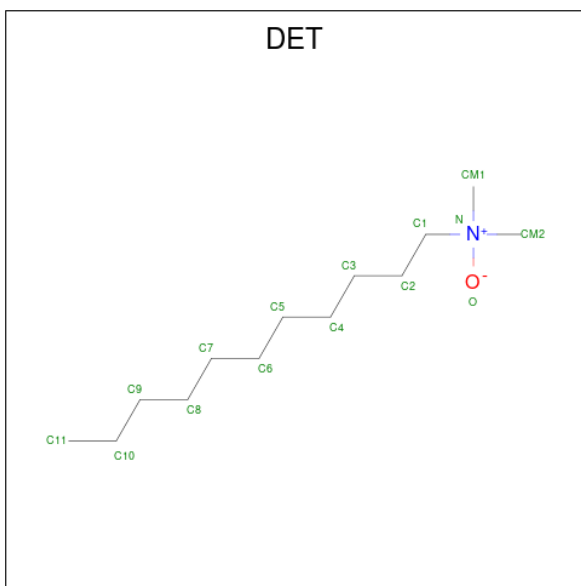
- Molecule 2 is 1-methyl-5-(2'-methyl[1,1'-biphenyl]-4-yl)-1H-benzotriazole-7-carboxylic acid (three-letter code: R4P) (formula: $C_{21}H_{17}N_3O_2$) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	1
			52	42	6	4		

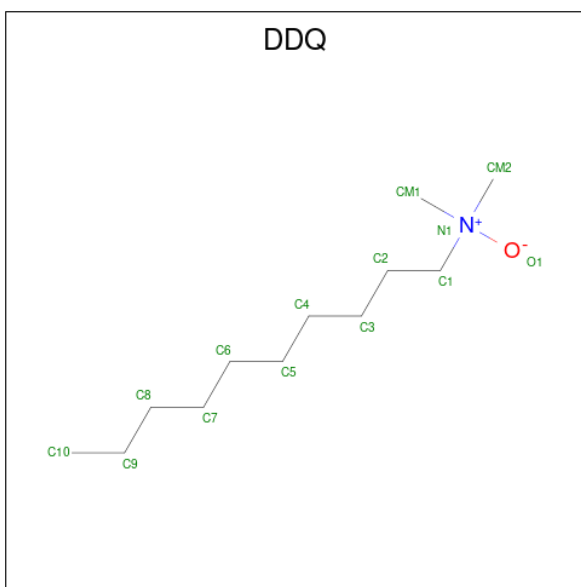
- Molecule 3 is UNDECYLAMINE-N,N-DIMETHYL-N-OXIDE (three-letter code: DET)

(formula: $C_{13}H_{29}NO$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			15	13	1	1		
3	A	1	Total	C	N	O	0	0
			15	13	1	1		

- Molecule 4 is DECYLAMINE-N,N-DIMETHYL-N-OXIDE (three-letter code: DDQ) (formula: $C_{12}H_{27}NO$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total 14	C 12	N 1	O 1	0	0
4	A	1	Total 28	C 24	N 2	O 2	0	1

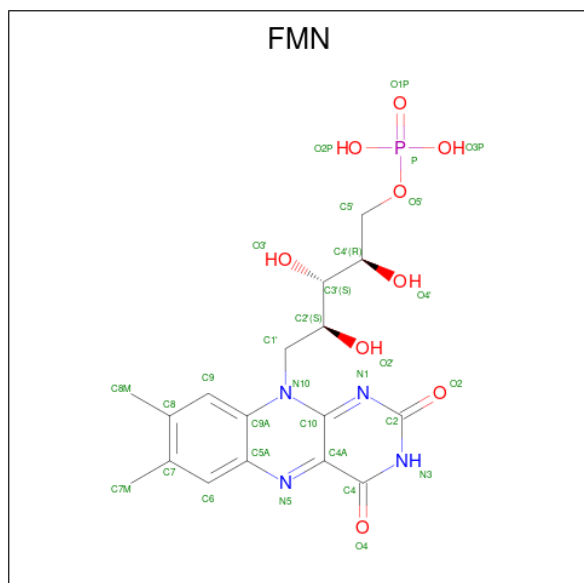
- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Cl 1 1	0	0

- Molecule 6 is SODIUM ION (three-letter code: NA) (formula: Na).

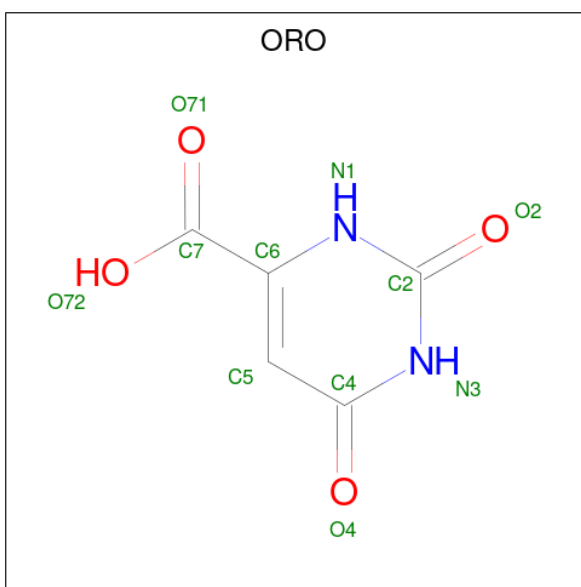
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	3	Total 3	Na 3	0	0

- Molecule 7 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: $\text{C}_{17}\text{H}_{21}\text{N}_4\text{O}_9\text{P}$).



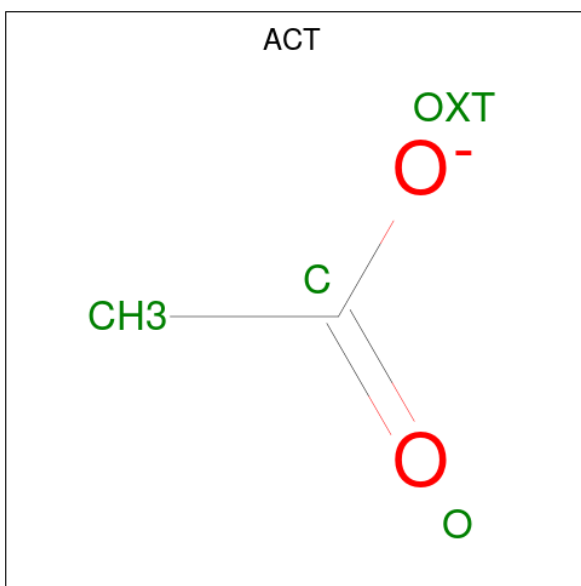
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	A	1	Total	C	N	O	P	0	0
			31	17	4	9	1		

- Molecule 8 is OROTIC ACID (three-letter code: ORO) (formula: $C_5H_4N_2O_4$).



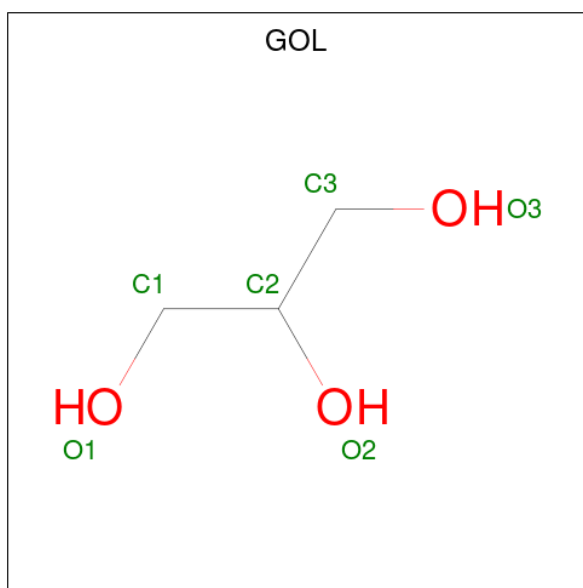
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total	C	N	O	0	0
			11	5	2	4		

- Molecule 9 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



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

- Molecule 10 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

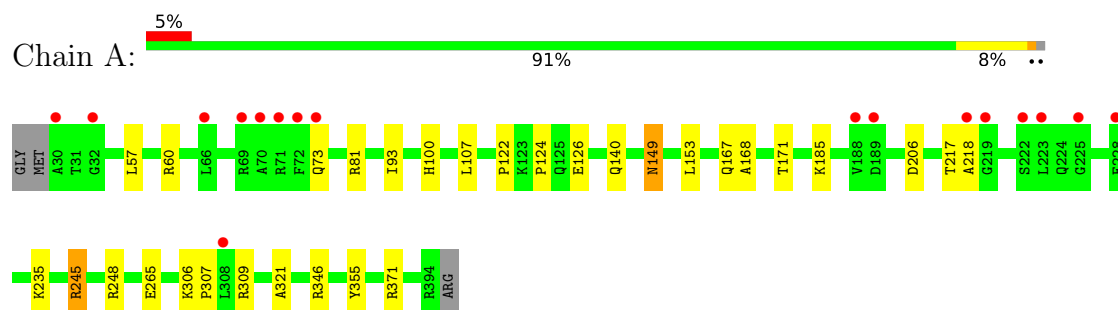
- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	228	Total	O	0	0
			228	228		

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 (quinone), mitochondrial



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	90.53Å 90.53Å 123.76Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	28.78 – 1.97 48.57 – 1.97	Depositor EDS
% Data completeness (in resolution range)	92.7 (28.78-1.97) 92.7 (48.57-1.97)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.82 (at 1.97Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.155 , 0.190 0.156 , 0.192	Depositor DCC
R_{free} test set	1885 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å ²)	28.8	Xtriage
Anisotropy	0.120	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 72.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.024 for -h,-k,l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	3256	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.03% 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: GOL, CL, NA, DDQ, DET, FMN, ORO, R4P, ACT

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.88	1/2875 (0.0%)	0.78	1/3887 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	265	GLU	CD-OE2	5.26	1.31	1.25

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	309	ARG	NE-CZ-NH1	-5.36	117.62	120.30

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	2810	0	2888	28	0
2	A	52	0	0	1	0
3	A	30	0	58	7	0
4	A	42	0	81	3	0
5	A	1	0	0	0	0
6	A	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	31	0	19	0	0
8	A	11	0	3	0	0
9	A	12	0	9	0	0
10	A	36	0	48	9	0
11	A	228	0	0	5	0
All	All	3256	0	3106	31	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 (31) 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:346:ARG:HH12	4:A:405[B]:DDQ:H41	1.52	0.75
1:A:307:PRO:HA	3:A:403:DET:H21	1.70	0.73
1:A:100:HIS:NE2	3:A:402:DET:H11	2.09	0.68
1:A:321:ALA:HA	10:A:419:GOL:H32	1.76	0.66
1:A:81:ARG:NH2	11:A:503:HOH:O	2.30	0.64
1:A:346:ARG:HH12	4:A:405[A]:DDQ:H41	1.63	0.63
1:A:149:ASN:HD22	1:A:149:ASN:H	1.52	0.57
1:A:206:ASP:OD1	10:A:417:GOL:O1	2.19	0.54
1:A:245:ARG:NE	1:A:245:ARG:H	2.07	0.53
1:A:245:ARG:HD3	1:A:248:ARG:NH2	2.24	0.51
3:A:403:DET:HM11	11:A:542:HOH:O	2.12	0.49
1:A:167:GLN:CG	10:A:417:GOL:H32	2.43	0.48
1:A:185:LYS:HD2	1:A:217[A]:THR:HG23	1.96	0.47
1:A:185:LYS:HE3	1:A:218:ALA:H	1.78	0.47
1:A:371:ARG:HD3	11:A:558:HOH:O	2.13	0.47
1:A:168:ALA:HA	10:A:417:GOL:H11	1.98	0.46
1:A:171:THR:OG1	10:A:417:GOL:H12	2.16	0.46
1:A:167:GLN:HG3	10:A:417:GOL:H32	1.98	0.46
1:A:167:GLN:HB3	10:A:417:GOL:H32	1.97	0.45
1:A:306:LYS:CG	3:A:403:DET:H81	2.46	0.45
1:A:124:PRO:HB2	3:A:402:DET:H102	1.98	0.45
1:A:122:PRO:HA	1:A:153:LEU:HG	1.99	0.45
1:A:60:ARG:NE	1:A:60:ARG:HA	2.31	0.44
1:A:57[B]:LEU:HG	4:A:404:DDQ:H101	1.99	0.44
1:A:126:GLU:HG2	3:A:402:DET:H113	1.99	0.43
1:A:140:GLN:HG3	3:A:403:DET:C10	2.48	0.43
1:A:235:LYS:NZ	11:A:510:HOH:O	2.53	0.42
2:A:401[A]:R4P:O1	2:A:401[A]:R4P:C14	2.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:419:GOL:H31	11:A:550:HOH:O	2.18	0.42
1:A:167:GLN:CB	10:A:417:GOL:H32	2.50	0.41
1:A:93:ILE:HG21	1:A:107:LEU:HD13	2.03	0.41

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	369/368 (100%)	356 (96%)	13 (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	300/296 (101%)	296 (99%)	4 (1%)	69 64

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	73	GLN
1	A	149	ASN
1	A	245	ARG

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Mol	Chain	Res	Type
1	A	355	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 22 ligands modelled in this entry, 4 are monoatomic - leaving 18 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	$\# Z > 2$
8	ORO	A	411	-	6,11,11	2.00	1 (16%)	3,15,15	4.98	2 (66%)
7	FMN	A	410	-	31,33,33	1.85	6 (19%)	40,50,50	2.65	6 (15%)
10	GOL	A	418	-	5,5,5	0.14	0	5,5,5	0.23	0
9	ACT	A	413	-	1,3,3	5.88	1 (100%)	0,3,3	0.00	-
9	ACT	A	414	-	1,3,3	5.90	1 (100%)	0,3,3	0.00	-
4	DDQ	A	405[B]	-	10,13,13	0.37	0	12,15,15	0.55	0
2	R4P	A	401[B]	-	24,29,29	1.83	4 (16%)	29,42,42	1.27	3 (10%)
9	ACT	A	412	-	1,3,3	4.96	1 (100%)	0,3,3	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	R4P	A	401[A]	-	24,29,29	1.67	4 (16%)	29,42,42	1.82	8 (27%)
10	GOL	A	416	-	5,5,5	0.48	0	5,5,5	0.59	0
10	GOL	A	417	-	5,5,5	0.37	0	5,5,5	0.55	0
4	DDQ	A	405[A]	-	10,13,13	0.37	0	12,15,15	0.67	1 (8%)
4	DDQ	A	404	-	10,13,13	0.38	0	12,15,15	0.43	0
10	GOL	A	415	-	5,5,5	0.18	0	5,5,5	0.36	0
3	DET	A	403	-	11,14,14	0.48	0	13,16,16	0.45	0
10	GOL	A	419	-	5,5,5	0.08	0	5,5,5	0.21	0
10	GOL	A	420	-	5,5,5	0.14	0	5,5,5	0.16	0
3	DET	A	402	6	11,14,14	0.44	0	13,16,16	1.24	2 (15%)

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
8	ORO	A	411	-	-	0/0/4/4	0/1/1/1
7	FMN	A	410	-	-	4/18/18/18	0/3/3/3
10	GOL	A	418	-	-	0/4/4/4	-
4	DDQ	A	404	-	-	4/11/11/11	-
4	DDQ	A	405[B]	-	-	5/11/11/11	-
2	R4P	A	401[B]	-	-	0/8/12/12	0/4/4/4
10	GOL	A	417	-	-	0/4/4/4	-
2	R4P	A	401[A]	-	-	0/8/12/12	0/4/4/4
10	GOL	A	416	-	-	0/4/4/4	-
4	DDQ	A	405[A]	-	-	8/11/11/11	-
10	GOL	A	415	-	-	3/4/4/4	-
3	DET	A	403	-	-	7/12/12/12	-
10	GOL	A	419	-	-	2/4/4/4	-
10	GOL	A	420	-	-	2/4/4/4	-
3	DET	A	402	6	-	7/12/12/12	-

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	410	FMN	C4A-C10	6.80	1.45	1.38
9	A	414	ACT	CH3-C	5.90	1.56	1.48
9	A	413	ACT	CH3-C	5.88	1.56	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401[B]	R4P	C1-C	5.35	1.52	1.47
9	A	412	ACT	CH3-C	4.96	1.55	1.48
2	A	401[B]	R4P	C1B-C1A	-4.95	1.40	1.49
2	A	401[A]	R4P	C1B-C1A	-4.83	1.40	1.49
8	A	411	ORO	C4-N3	4.08	1.40	1.33
2	A	401[A]	R4P	C16-C17	-4.07	1.38	1.49
2	A	401[B]	R4P	C16-C17	-3.98	1.39	1.49
7	A	410	FMN	C9A-N10	3.62	1.43	1.38
7	A	410	FMN	C5A-N5	3.37	1.40	1.35
2	A	401[A]	R4P	N1-N12	3.35	1.41	1.34
7	A	410	FMN	P-O5'	2.79	1.69	1.60
7	A	410	FMN	C4-N3	2.77	1.37	1.33
7	A	410	FMN	C4-C4A	2.61	1.45	1.41
2	A	401[A]	R4P	C1-C	2.29	1.49	1.47
2	A	401[B]	R4P	N1-N12	2.03	1.38	1.34

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	410	FMN	C4-N3-C2	12.60	125.78	115.14
8	A	411	ORO	C5-C4-N3	-7.27	115.60	124.08
7	A	410	FMN	C4A-C4-N3	-6.67	114.31	123.43
7	A	410	FMN	C10-C4A-N5	4.56	124.41	121.26
8	A	411	ORO	C4-C5-C6	4.56	119.67	116.73
7	A	410	FMN	C4A-C10-N10	-4.05	116.14	120.30
7	A	410	FMN	C4-C4A-C10	-3.97	117.33	119.95
2	A	401[A]	R4P	C15-C13-C12	-3.79	117.30	121.12
2	A	401[A]	R4P	C16-C15-C13	3.52	124.51	121.44
2	A	401[A]	R4P	C1A-C1B-C1G	3.32	129.26	122.48
3	A	402	DET	CM2-N-C1	-3.13	103.65	110.23
2	A	401[B]	R4P	C14-N12-N1	3.09	121.91	117.67
7	A	410	FMN	C1'-N10-C9A	3.08	120.72	118.29
3	A	402	DET	CM1-N-C1	3.06	116.67	110.23
2	A	401[A]	R4P	C1K-C16-C17	2.97	125.77	120.86
2	A	401[B]	R4P	C1I-C1A-C1B	-2.94	116.14	120.91
2	A	401[A]	R4P	C1C-C1B-C1A	-2.85	113.05	118.68
2	A	401[A]	R4P	C15-C16-C17	-2.84	114.56	121.05
2	A	401[A]	R4P	C12-C13-N	2.67	111.81	108.63
2	A	401[A]	R4P	C14-N12-N1	2.64	121.30	117.67
2	A	401[B]	R4P	C19-C1A-C1B	2.55	125.04	120.91
4	A	405[A]	DDQ	CM2-N1-C1	-2.07	105.88	110.23

There are no chirality outliers.

All (42) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	405[B]	DDQ	C2-C1-N1-O1
4	A	405[B]	DDQ	C2-C1-N1-CM2
4	A	405[A]	DDQ	C2-C1-N1-O1
4	A	405[A]	DDQ	C2-C1-N1-CM2
10	A	415	GOL	O1-C1-C2-C3
3	A	403	DET	C2-C1-N-O
3	A	403	DET	C2-C1-N-CM2
3	A	403	DET	N-C1-C2-C3
4	A	404	DDQ	N1-C1-C2-C3
3	A	402	DET	C2-C1-N-CM2
4	A	405[B]	DDQ	C6-C7-C8-C9
7	A	410	FMN	O3'-C3'-C4'-O4'
3	A	403	DET	C6-C7-C8-C9
7	A	410	FMN	C2'-C3'-C4'-O4'
3	A	403	DET	C4-C5-C6-C7
10	A	415	GOL	C1-C2-C3-O3
10	A	420	GOL	C1-C2-C3-O3
3	A	402	DET	C5-C6-C7-C8
4	A	404	DDQ	C5-C6-C7-C8
10	A	415	GOL	O1-C1-C2-O2
4	A	404	DDQ	C1-C2-C3-C4
4	A	405[A]	DDQ	C5-C6-C7-C8
3	A	402	DET	C1-C2-C3-C4
4	A	404	DDQ	C2-C3-C4-C5
3	A	403	DET	C1-C2-C3-C4
10	A	420	GOL	O2-C2-C3-O3
4	A	405[A]	DDQ	C7-C8-C9-C10
10	A	419	GOL	C1-C2-C3-O3
4	A	405[A]	DDQ	C3-C4-C5-C6
4	A	405[B]	DDQ	C3-C4-C5-C6
3	A	402	DET	C6-C7-C8-C9
4	A	405[B]	DDQ	C1-C2-C3-C4
3	A	402	DET	C3-C4-C5-C6
3	A	403	DET	C2-C1-N-CM1
3	A	402	DET	C2-C1-N-CM1
7	A	410	FMN	C4'-C5'-O5'-P
7	A	410	FMN	O3'-C3'-C4'-C5'
4	A	405[A]	DDQ	C1-C2-C3-C4
4	A	405[A]	DDQ	C4-C5-C6-C7
4	A	405[A]	DDQ	C6-C7-C8-C9

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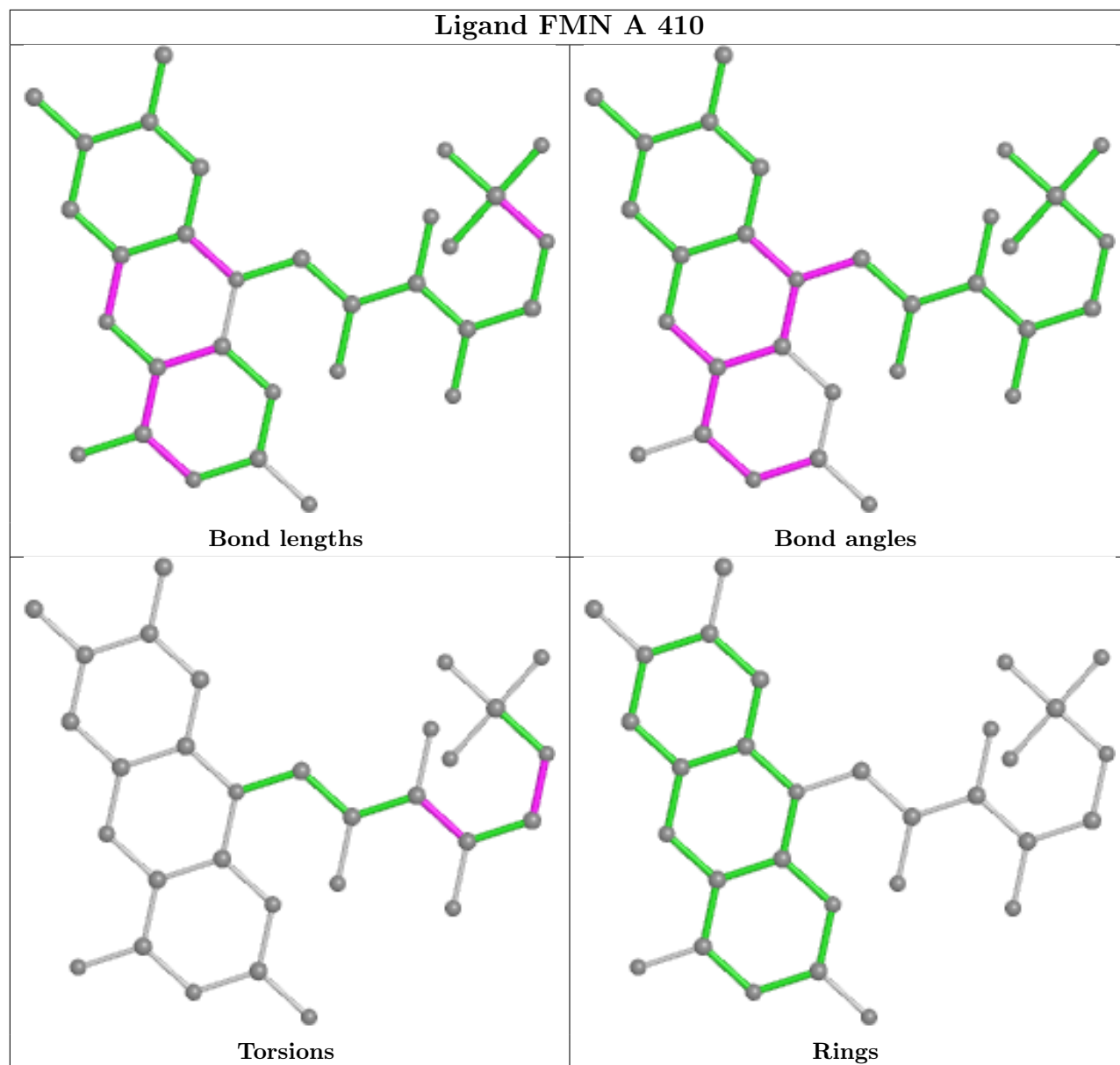
Mol	Chain	Res	Type	Atoms
3	A	402	DET	C4-C5-C6-C7
10	A	419	GOL	O1-C1-C2-C3

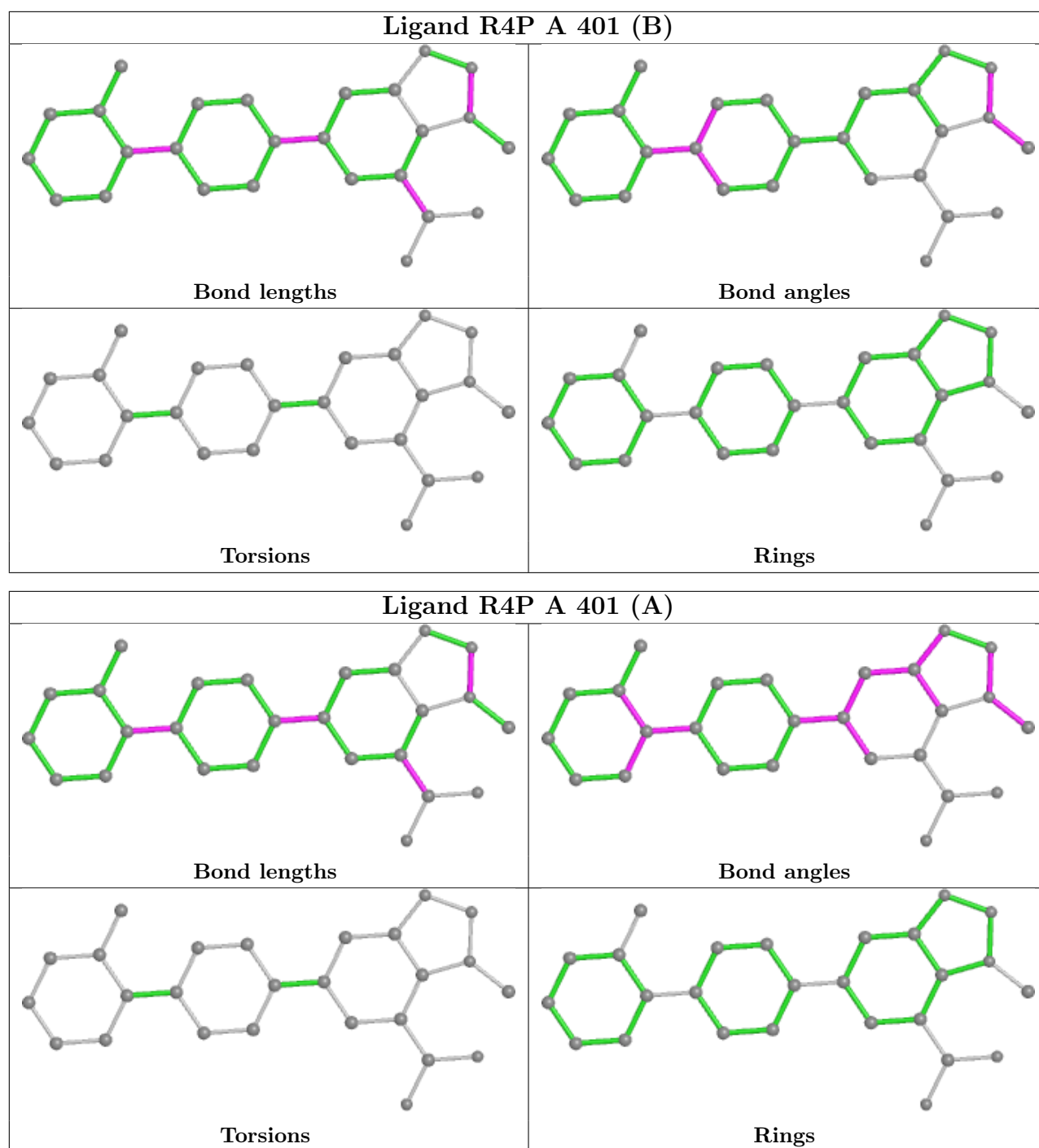
There are no ring outliers.

8 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	405[B]	DDQ	1	0
2	A	401[A]	R4P	1	0
10	A	417	GOL	7	0
4	A	405[A]	DDQ	1	0
4	A	404	DDQ	1	0
3	A	403	DET	4	0
10	A	419	GOL	2	0
3	A	402	DET	3	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	365/368 (99%)	-0.19	17 (4%) 31 33	19, 30, 58, 121	1 (0%)

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	71	ARG	8.8
1	A	69	ARG	5.6
1	A	72	PHE	5.3
1	A	188	VAL	4.6
1	A	73	GLN	3.9
1	A	70	ALA	3.8
1	A	218	ALA	3.6
1	A	30	ALA	3.3
1	A	222	SER	3.1
1	A	189	ASP	3.0
1	A	219	GLY	2.8
1	A	32	GLY	2.7
1	A	228	GLU	2.6
1	A	223	LEU	2.5
1	A	308	LEU	2.5
1	A	66	LEU	2.3
1	A	225	GLY	2.1

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 ⓘ

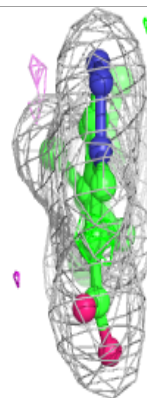
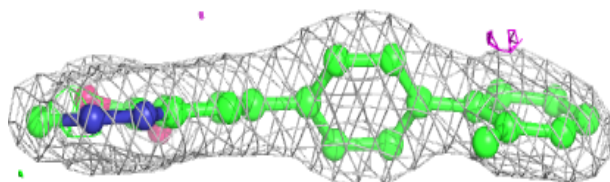
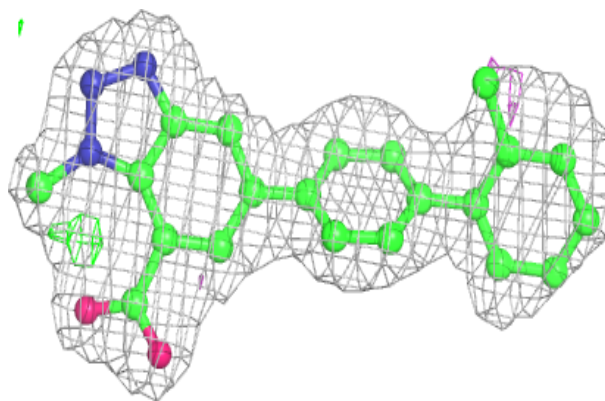
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
10	GOL	A	418	6/6	0.80	0.32	78,80,82,85	0
3	DET	A	402	15/15	0.82	0.21	50,63,71,78	0
10	GOL	A	416	6/6	0.82	0.20	47,56,61,66	0
10	GOL	A	415	6/6	0.85	0.22	52,62,69,71	0
3	DET	A	403	15/15	0.85	0.35	37,50,76,83	0
4	DDQ	A	405[B]	14/14	0.85	0.21	44,55,64,69	14
4	DDQ	A	405[A]	14/14	0.85	0.21	45,55,64,68	14
9	ACT	A	413	4/4	0.87	0.17	63,63,72,74	0
9	ACT	A	414	4/4	0.87	0.16	64,69,74,77	0
4	DDQ	A	404	14/14	0.88	0.30	56,65,76,81	0
10	GOL	A	420	6/6	0.88	0.20	70,75,76,78	0
6	NA	A	409	1/1	0.88	0.15	70,70,70,70	0
10	GOL	A	417	6/6	0.89	0.12	34,48,52,63	0
6	NA	A	407	1/1	0.90	0.35	84,84,84,84	0
6	NA	A	408	1/1	0.92	0.23	61,61,61,61	0
9	ACT	A	412	4/4	0.93	0.15	48,53,55,57	0
5	CL	A	406	1/1	0.95	0.06	53,53,53,53	0
10	GOL	A	419	6/6	0.96	0.11	67,69,73,78	0
2	R4P	A	401[B]	26/26	0.97	0.08	25,30,37,42	26
2	R4P	A	401[A]	26/26	0.97	0.08	24,30,39,47	26
8	ORO	A	411	11/11	0.98	0.06	20,22,29,29	0
7	FMN	A	410	31/31	0.99	0.09	17,21,23,24	0

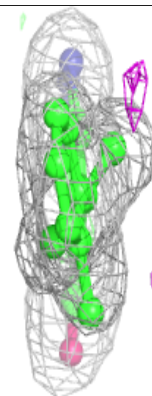
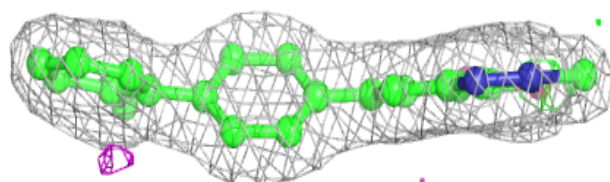
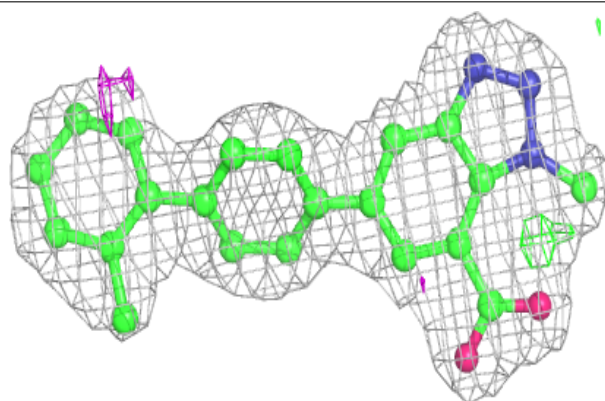
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around R4P A 401 (B):

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

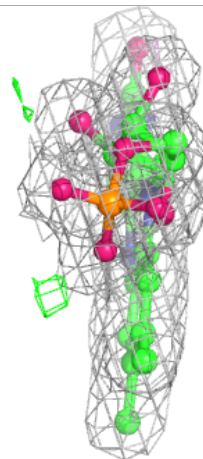
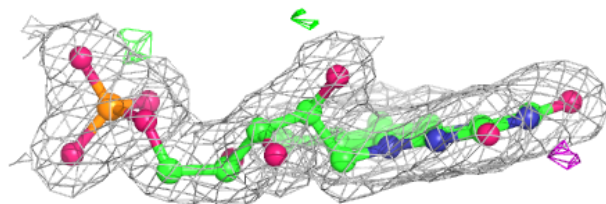
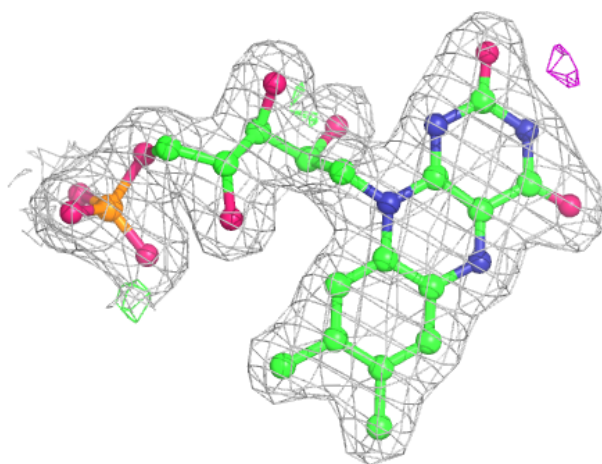
**Electron density around R4P A 401 (A):**

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



Electron density around FMN A 410:

$2mF_o-DF_c$ (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.