Full wwPDB X-ray Structure Validation Report (i)

Sep 18, 2023 – 01:57 PM EDT

PDB ID	:	5BOO
Title	:	Crystal structure of Plasmodium falciparum dihydroorotate dehydrogenase bound with Inhibitor DSM265
Authors	:	Phillips, M.; Deng, X.; Tomchick, D.
Deposited on	:	2015-05-27
Resolution	:	2.80 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 (i) 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 (i)) were used in the production of this report:

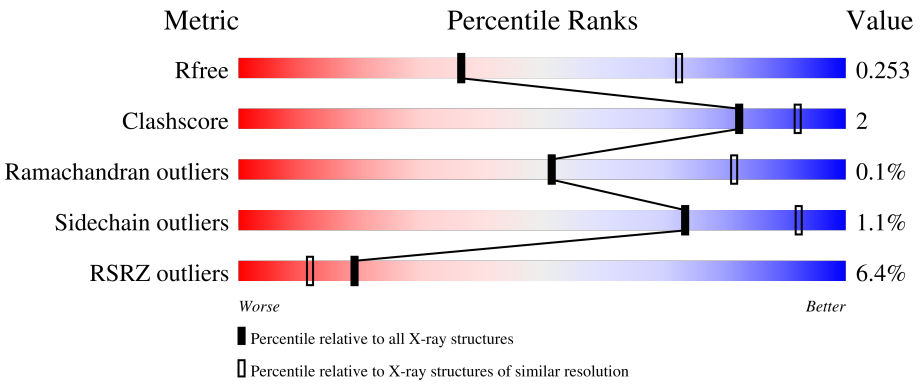
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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 <=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	415	4% 82% 7% 10%
1	B	415	8% 86% • 10%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 12128 atoms, of which 6075 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
			Total	C	H	N	O	S			
1	A	374	5972	1893	3010	496	558	15	0	0	0
1	B	373	5950	1887	2997	494	557	15	0	0	0

There are 126 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	125	MET	-	expression tag	UNP Q08210
A	126	GLY	-	expression tag	UNP Q08210
A	127	SER	-	expression tag	UNP Q08210
A	128	SER	-	expression tag	UNP Q08210
A	129	HIS	-	expression tag	UNP Q08210
A	130	HIS	-	expression tag	UNP Q08210
A	131	HIS	-	expression tag	UNP Q08210
A	132	HIS	-	expression tag	UNP Q08210
A	133	HIS	-	expression tag	UNP Q08210
A	134	HIS	-	expression tag	UNP Q08210
A	135	SER	-	expression tag	UNP Q08210
A	136	SER	-	expression tag	UNP Q08210
A	137	GLY	-	expression tag	UNP Q08210
A	138	LEU	-	expression tag	UNP Q08210
A	139	VAL	-	expression tag	UNP Q08210
A	140	PRO	-	expression tag	UNP Q08210
A	141	ARG	-	expression tag	UNP Q08210
A	142	GLY	-	expression tag	UNP Q08210
A	143	SER	-	expression tag	UNP Q08210
A	144	HIS	-	expression tag	UNP Q08210
A	145	MET	-	expression tag	UNP Q08210
A	146	ALA	-	expression tag	UNP Q08210
A	147	SER	-	expression tag	UNP Q08210
A	148	MET	-	expression tag	UNP Q08210
A	149	THR	-	expression tag	UNP Q08210

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Chain	Residue	Modelled	Actual	Comment	Reference
A	150	GLY	-	expression tag	UNP Q08210
A	151	GLY	-	expression tag	UNP Q08210
A	152	GLN	-	expression tag	UNP Q08210
A	153	GLN	-	expression tag	UNP Q08210
A	154	GLY	-	expression tag	UNP Q08210
A	155	ARG	-	expression tag	UNP Q08210
A	156	ASP	-	expression tag	UNP Q08210
A	157	PRO	-	expression tag	UNP Q08210
A	?	-	SER	deletion	UNP Q08210
A	?	-	THR	deletion	UNP Q08210
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	125	MET	-	expression tag	UNP Q08210
B	126	GLY	-	expression tag	UNP Q08210
B	127	SER	-	expression tag	UNP Q08210
B	128	SER	-	expression tag	UNP Q08210

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Chain	Residue	Modelled	Actual	Comment	Reference
B	129	HIS	-	expression tag	UNP Q08210
B	130	HIS	-	expression tag	UNP Q08210
B	131	HIS	-	expression tag	UNP Q08210
B	132	HIS	-	expression tag	UNP Q08210
B	133	HIS	-	expression tag	UNP Q08210
B	134	HIS	-	expression tag	UNP Q08210
B	135	SER	-	expression tag	UNP Q08210
B	136	SER	-	expression tag	UNP Q08210
B	137	GLY	-	expression tag	UNP Q08210
B	138	LEU	-	expression tag	UNP Q08210
B	139	VAL	-	expression tag	UNP Q08210
B	140	PRO	-	expression tag	UNP Q08210
B	141	ARG	-	expression tag	UNP Q08210
B	142	GLY	-	expression tag	UNP Q08210
B	143	SER	-	expression tag	UNP Q08210
B	144	HIS	-	expression tag	UNP Q08210
B	145	MET	-	expression tag	UNP Q08210
B	146	ALA	-	expression tag	UNP Q08210
B	147	SER	-	expression tag	UNP Q08210
B	148	MET	-	expression tag	UNP Q08210
B	149	THR	-	expression tag	UNP Q08210
B	150	GLY	-	expression tag	UNP Q08210
B	151	GLY	-	expression tag	UNP Q08210
B	152	GLN	-	expression tag	UNP Q08210
B	153	GLN	-	expression tag	UNP Q08210
B	154	GLY	-	expression tag	UNP Q08210
B	155	ARG	-	expression tag	UNP Q08210
B	156	ASP	-	expression tag	UNP Q08210
B	157	PRO	-	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

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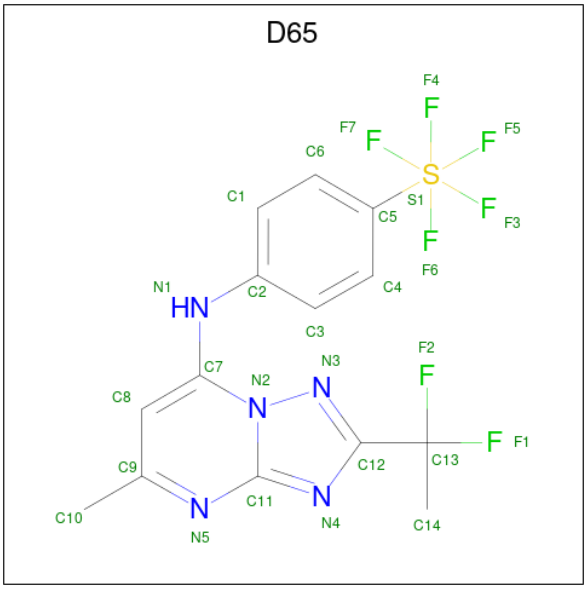
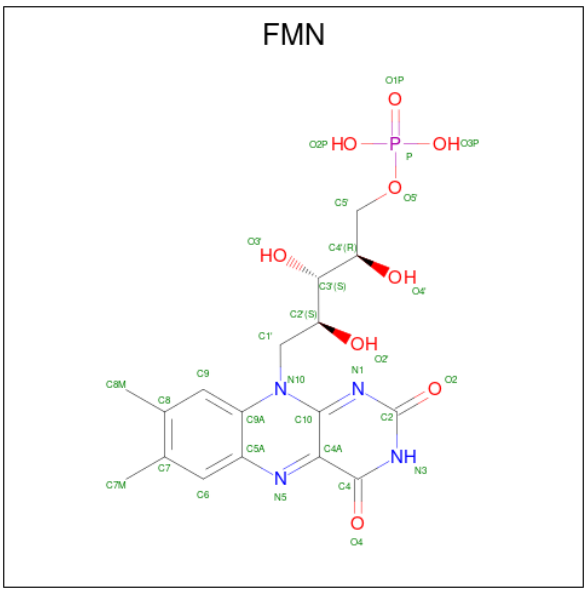
Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	ASN	deletion	UNP Q08210
B	?	-	ASN	deletion	UNP Q08210
B	?	-	PHE	deletion	UNP Q08210
B	?	-	ASN	deletion	UNP Q08210
B	?	-	LYS	deletion	UNP Q08210
B	?	-	ASN	deletion	UNP Q08210
B	?	-	ASN	deletion	UNP Q08210
B	?	-	SER	deletion	UNP Q08210
B	?	-	HIS	deletion	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 2-(1,1-difluoroethyl)-5-methyl-N-[4-(pentafluoro-lambda 6 -sulfanyl)phenyl][1,2,4]triazolo[1,5-a]pyrimidin-7-amine (three-letter code: D65) (formula: $C_{14}H_{12}F_7N_5S$).



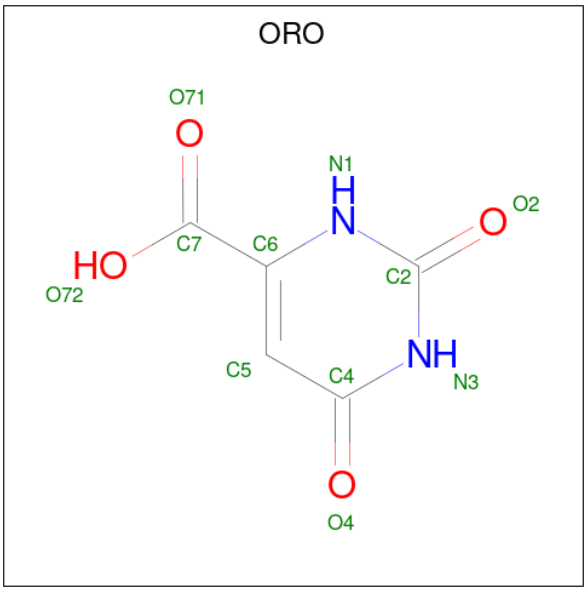
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	F	H	N	S		
2	A	1	39	14	7	12	5	1	0	0
			Total	C	F	H	N	S		
2	B	1	39	14	7	12	5	1	0	0

- Molecule 3 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: $C_{17}H_{21}N_4O_9P$).



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

- Molecule 4 is OROTIC ACID (three-letter code: ORO) (formula: $C_5H_4N_2O_4$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	H	N	O		
4	A	1	14	5	3	2	4	0	0

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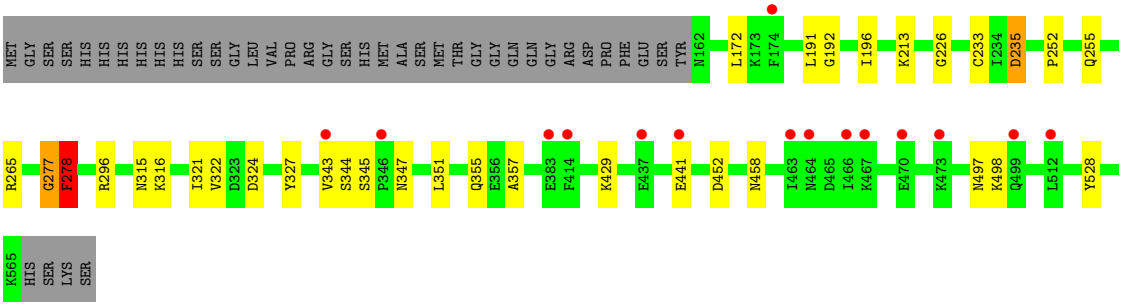
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	H	N	O		
4	B	1	14	5	3	2	4	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

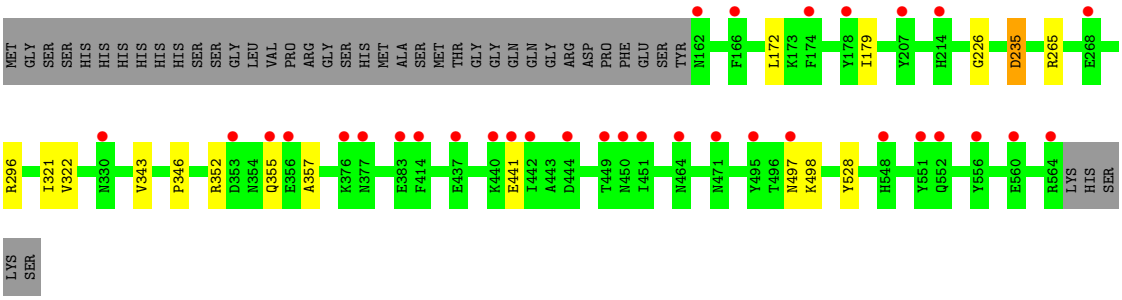
• Molecule 1: Dihydroorotate dehydrogenase (quinone), mitochondrial

Chain A:



• Molecule 1: Dihydroorotate dehydrogenase (quinone), mitochondrial

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α, β, γ	89.26Å 89.26Å 275.61Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	44.10 – 2.80 44.05 – 2.79	Depositor EDS
% Data completeness (in resolution range)	88.7 (44.10-2.80) 88.7 (44.05-2.79)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.13 (at 2.77Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.234 , 0.254 0.237 , 0.253	Depositor DCC
R_{free} test set	1988 reflections (7.27%)	wwPDB-VP
Wilson B-factor (Å^2)	44.0	Xtriage
Anisotropy	0.074	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 42.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.063 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	12128	wwPDB-VP
Average B, all atoms (Å^2)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.49% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: ORO, FMN, D65

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	0.27	0/3011	0.51	0/4054
1	B	0.26	0/3002	0.49	0/4043
All	All	0.27	0/6013	0.50	0/8097

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	A	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	277	GLY	Peptide

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	2962	3010	3010	21	0
1	B	2953	2997	2997	9	0
2	A	27	12	12	1	0
2	B	27	12	12	0	0
3	A	31	19	19	1	0
3	B	31	19	19	1	0
4	A	11	3	3	2	0
4	B	11	3	3	0	0
All	All	6053	6075	6075	30	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 2.

All (30) 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:277:GLY:HA2	1:A:347:ASN:HB3	1.81	0.63
1:B:497:ASN:O	1:B:498:LYS:HG2	2.02	0.60
1:A:343:VAL:HG23	1:A:355:GLN:HG2	1.85	0.59
1:A:344:SER:O	1:A:458:ASN:ND2	2.37	0.57
1:A:497:ASN:O	1:A:498:LYS:HG2	2.05	0.55
1:A:235:ASP:OD1	1:A:296:ARG:NH1	2.41	0.53
1:B:179:ILE:O	1:B:265:ARG:NH2	2.33	0.50
1:B:321:ILE:HG23	1:B:322:VAL:N	2.29	0.47
1:B:343:VAL:HG23	1:B:355:GLN:HG2	1.97	0.47
1:A:277:GLY:O	1:A:278:PHE:HB2	2.15	0.46
1:A:345:SER:HB3	1:A:351:LEU:HD23	1.98	0.46
1:B:226:GLY:HA3	3:B:1002:FMN:N5	2.30	0.46
1:A:345:SER:HB3	1:A:351:LEU:CD2	2.46	0.46
1:A:226:GLY:HA3	3:A:1002:FMN:N5	2.32	0.45
1:A:321:ILE:HG23	1:A:322:VAL:N	2.31	0.45
1:A:278:PHE:CE1	4:A:1003:ORO:H5	2.52	0.44
1:B:235:ASP:OD1	1:B:296:ARG:NH1	2.49	0.44
1:A:357:ALA:HB2	1:A:441:GLU:HG2	2.00	0.43
1:A:265:ARG:HD3	2:A:1001:D65:N4	2.34	0.43
1:A:255:GLN:OE1	1:A:316:LYS:N	2.43	0.42
1:B:357:ALA:HB2	1:B:441:GLU:HG2	2.01	0.42
1:A:344:SER:OG	1:A:429:LYS:O	2.37	0.42
1:A:192:GLY:HA3	1:A:233:CYS:SG	2.60	0.42
1:A:278:PHE:HE1	4:A:1003:ORO:H5	1.85	0.42
1:A:252:PRO:HB3	1:A:327:TYR:CD2	2.55	0.41
1:A:315:ASN:N	1:A:324:ASP:OD2	2.47	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:346:PRO:HA	1:B:352:ARG:HD2	2.02	0.41
1:A:213:LYS:HE2	1:A:452:ASP:HA	2.03	0.41
1:A:191:LEU:HD22	1:A:196:ILE:HD11	2.02	0.41
1:B:235:ASP:OD1	1:B:235:ASP:N	2.52	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	372/415 (90%)	358 (96%)	13 (4%)	1 (0%)	41 72
1	B	371/415 (89%)	358 (96%)	13 (4%)	0	100 100
All	All	743/830 (90%)	716 (96%)	26 (4%)	1 (0%)	51 81

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	278	PHE

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	331/365 (91%)	327 (99%)	4 (1%)	71 92

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	330/365 (90%)	327 (99%)	3 (1%)	78 94
All	All	661/730 (90%)	654 (99%)	7 (1%)	73 92

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	172	LEU
1	A	235	ASP
1	A	278	PHE
1	A	528	TYR
1	B	172	LEU
1	B	235	ASP
1	B	528	TYR

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

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides 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	ORO	A	1003	-	9,11,11	1.03	0	8,15,15	2.80	4 (50%)
2	D65	B	1001	-	23,29,29	3.35	4 (17%)	39,51,51	1.29	4 (10%)
2	D65	A	1001	-	23,29,29	3.35	4 (17%)	39,51,51	1.35	4 (10%)
4	ORO	B	1003	-	9,11,11	1.08	0	8,15,15	2.52	4 (50%)
3	FMN	A	1002	-	33,33,33	1.04	2 (6%)	48,50,50	1.24	7 (14%)
3	FMN	B	1002	-	33,33,33	1.03	2 (6%)	48,50,50	1.23	7 (14%)

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	A	1003	-	-	4/4/4/4	0/1/1/1
2	D65	B	1001	-	-	2/18/20/20	0/3/3/3
2	D65	A	1001	-	-	4/18/20/20	0/3/3/3
4	ORO	B	1003	-	-	4/4/4/4	0/1/1/1
3	FMN	A	1002	-	-	3/18/18/18	0/3/3/3
3	FMN	B	1002	-	-	3/18/18/18	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1001	D65	C5-S1	-14.03	1.64	1.80
2	B	1001	D65	C5-S1	-13.98	1.64	1.80
2	B	1001	D65	F1-C13	-5.00	1.32	1.37
2	A	1001	D65	F1-C13	-4.85	1.32	1.37
2	A	1001	D65	F2-C13	-4.81	1.32	1.37
2	B	1001	D65	F2-C13	-4.76	1.32	1.37
3	A	1002	FMN	C4A-N5	3.87	1.38	1.30
3	B	1002	FMN	C4A-N5	3.66	1.37	1.30
3	A	1002	FMN	C10-N1	2.39	1.38	1.33
3	B	1002	FMN	C10-N1	2.36	1.38	1.33
2	A	1001	D65	C2-N1	-2.14	1.36	1.40
2	B	1001	D65	C2-N1	-2.14	1.36	1.40

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	1003	ORO	C6-C5-C4	5.46	120.26	116.73
2	A	1001	D65	C7-C8-C9	5.04	120.86	117.08
2	B	1001	D65	C7-C8-C9	4.63	120.56	117.08
4	B	1003	ORO	C6-C5-C4	4.59	119.70	116.73
4	A	1003	ORO	C5-C4-N3	-3.67	119.79	124.08
4	B	1003	ORO	C5-C4-N3	-3.39	120.13	124.08
3	A	1002	FMN	C4-N3-C2	-3.22	119.69	125.64
3	B	1002	FMN	C4-N3-C2	-3.05	120.00	125.64
3	A	1002	FMN	C4A-C10-N10	2.98	120.83	116.48
2	A	1001	D65	C8-C7-N1	2.90	127.76	123.36
3	B	1002	FMN	C4A-C10-N10	2.72	120.46	116.48
3	A	1002	FMN	C4A-C4-N3	2.64	119.91	113.19
4	A	1003	ORO	C7-C6-N1	2.63	120.36	116.48
2	B	1001	D65	C8-C7-N1	2.62	127.34	123.36
3	B	1002	FMN	C4A-C4-N3	2.56	119.69	113.19
3	B	1002	FMN	O4-C4-C4A	-2.48	120.01	126.60
4	B	1003	ORO	C7-C6-N1	2.48	120.14	116.48
4	B	1003	ORO	O72-C7-C6	2.44	120.24	114.69
4	A	1003	ORO	O72-C7-C6	2.41	120.17	114.69
3	A	1002	FMN	C4A-C10-N1	-2.40	119.17	124.73
3	A	1002	FMN	O4-C4-C4A	-2.39	120.26	126.60
3	A	1002	FMN	C10-C4A-N5	-2.38	119.80	124.86
3	B	1002	FMN	C4A-C10-N1	-2.31	119.36	124.73
3	B	1002	FMN	C10-C4A-N5	-2.16	120.28	124.86
2	B	1001	D65	F4-S1-F7	2.14	179.97	106.06
2	A	1001	D65	F6-S1-F3	2.14	179.95	106.06
2	A	1001	D65	F4-S1-F7	2.13	179.92	106.06
2	B	1001	D65	F6-S1-F3	2.13	179.92	106.06
3	B	1002	FMN	C4-C4A-C10	2.11	120.33	116.79
3	A	1002	FMN	C4-C4A-C10	2.04	120.22	116.79

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1001	D65	C4-C5-S1-F5
2	A	1001	D65	C6-C5-S1-F5
2	B	1001	D65	N3-C12-C13-F2
3	A	1002	FMN	C5'-O5'-P-O1P
3	A	1002	FMN	C5'-O5'-P-O2P
3	B	1002	FMN	C5'-O5'-P-O2P
3	B	1002	FMN	C5'-O5'-P-O3P
4	A	1003	ORO	N1-C6-C7-O71

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Mol	Chain	Res	Type	Atoms
4	A	1003	ORO	N1-C6-C7-O72
4	A	1003	ORO	C5-C6-C7-O71
4	A	1003	ORO	C5-C6-C7-O72
4	B	1003	ORO	N1-C6-C7-O71
4	B	1003	ORO	N1-C6-C7-O72
4	B	1003	ORO	C5-C6-C7-O71
4	B	1003	ORO	C5-C6-C7-O72
2	A	1001	D65	N3-C12-C13-F1
2	A	1001	D65	N3-C12-C13-F2
3	B	1002	FMN	C5'-O5'-P-O1P
2	B	1001	D65	N3-C12-C13-F1
3	A	1002	FMN	C5'-O5'-P-O3P

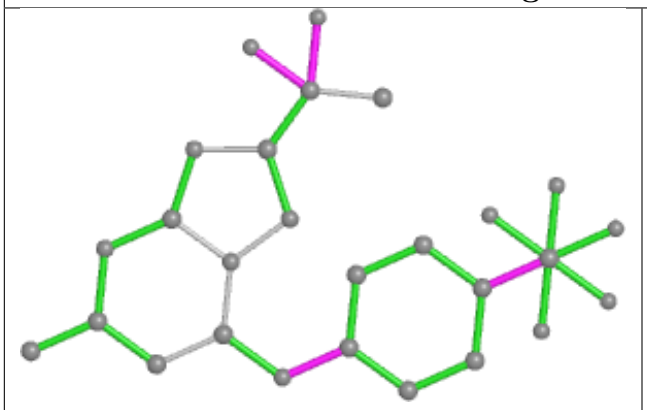
There are no ring outliers.

4 monomers are involved in 5 short contacts:

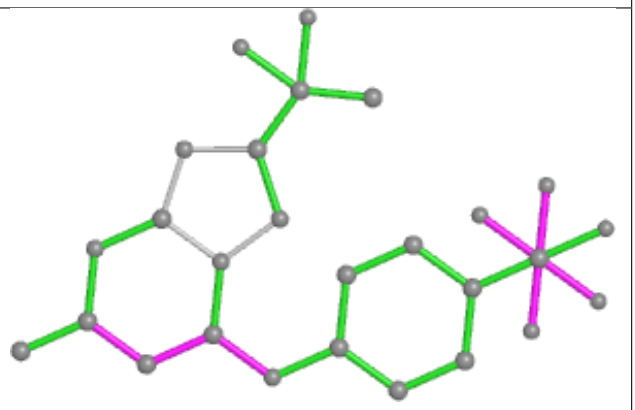
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1003	ORO	2	0
2	A	1001	D65	1	0
3	A	1002	FMN	1	0
3	B	1002	FMN	1	0

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 then 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.

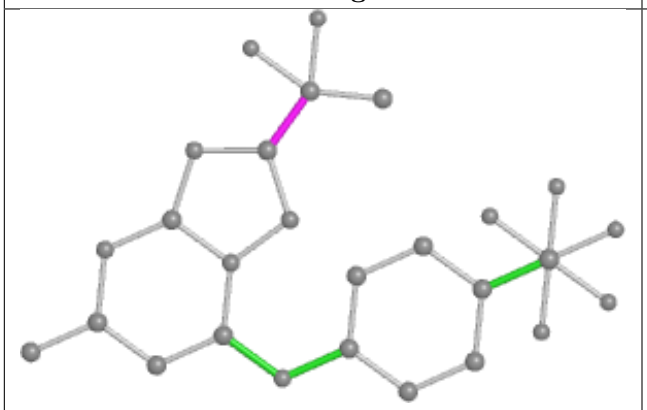
Ligand D65 B 1001



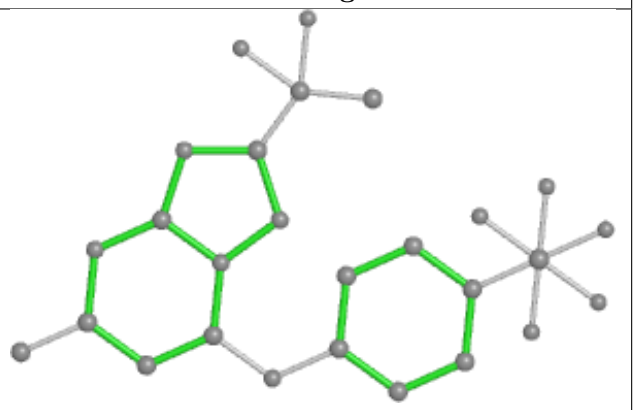
Bond lengths



Bond angles

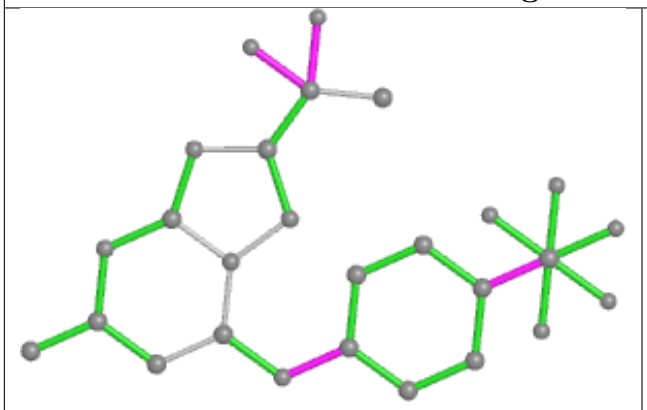


Torsions

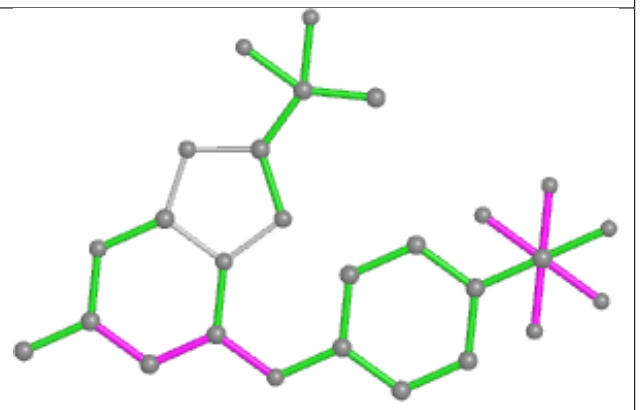


Rings

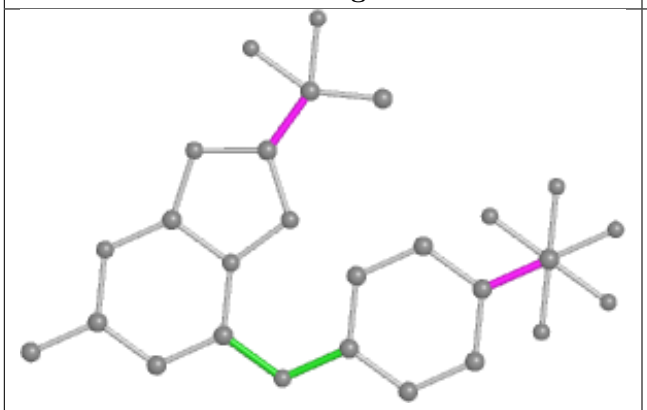
Ligand D65 A 1001



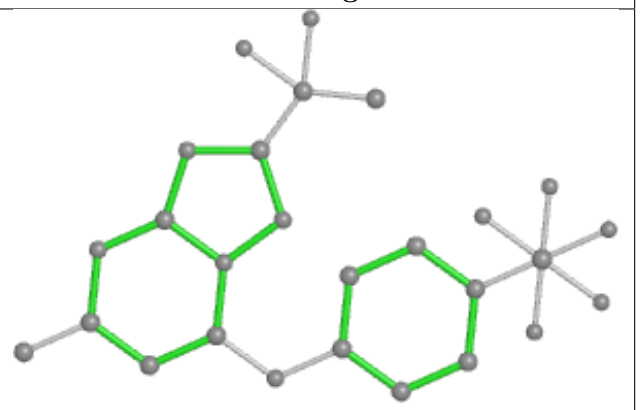
Bond lengths



Bond angles

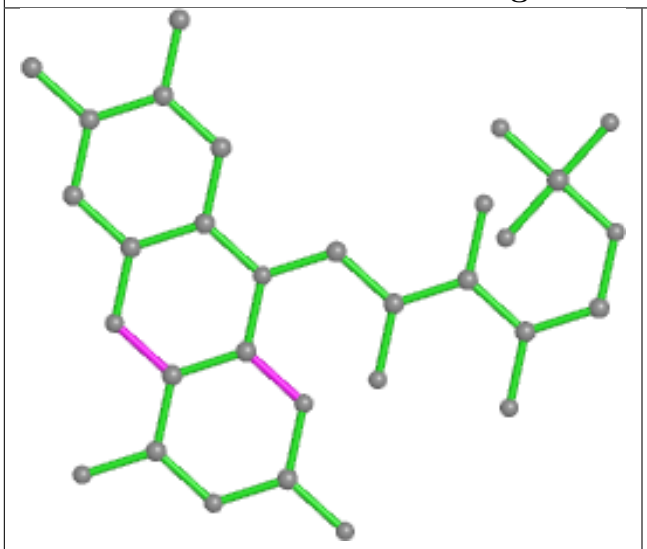


Torsions

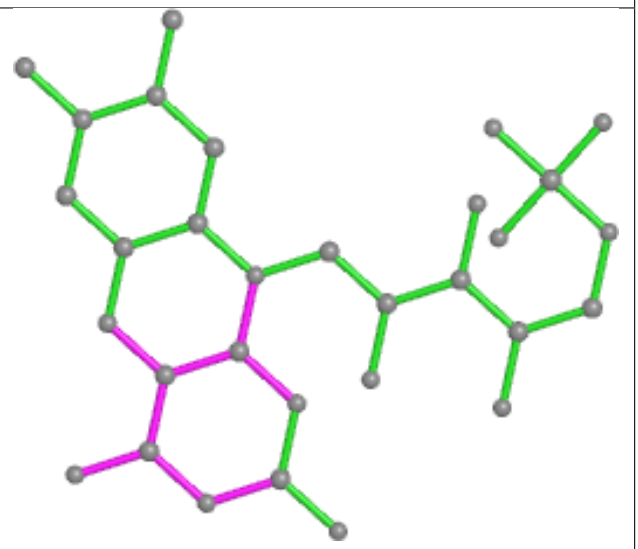


Rings

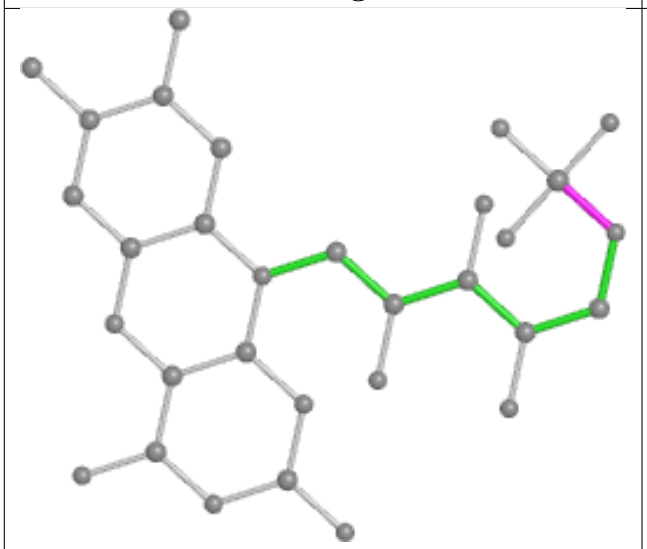
Ligand FMN A 1002



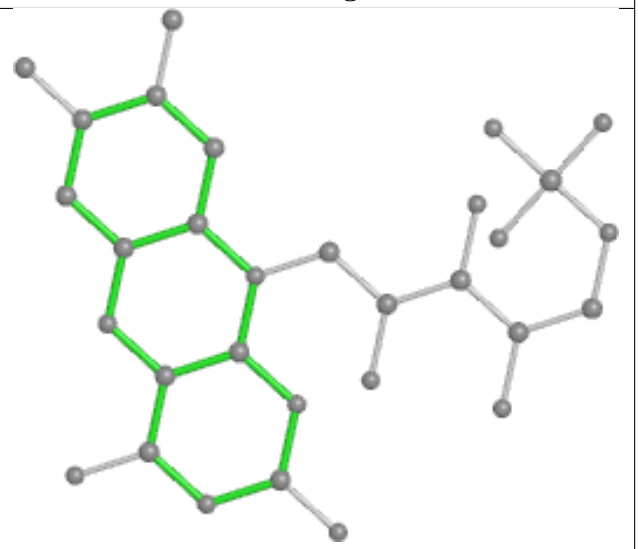
Bond lengths



Bond angles

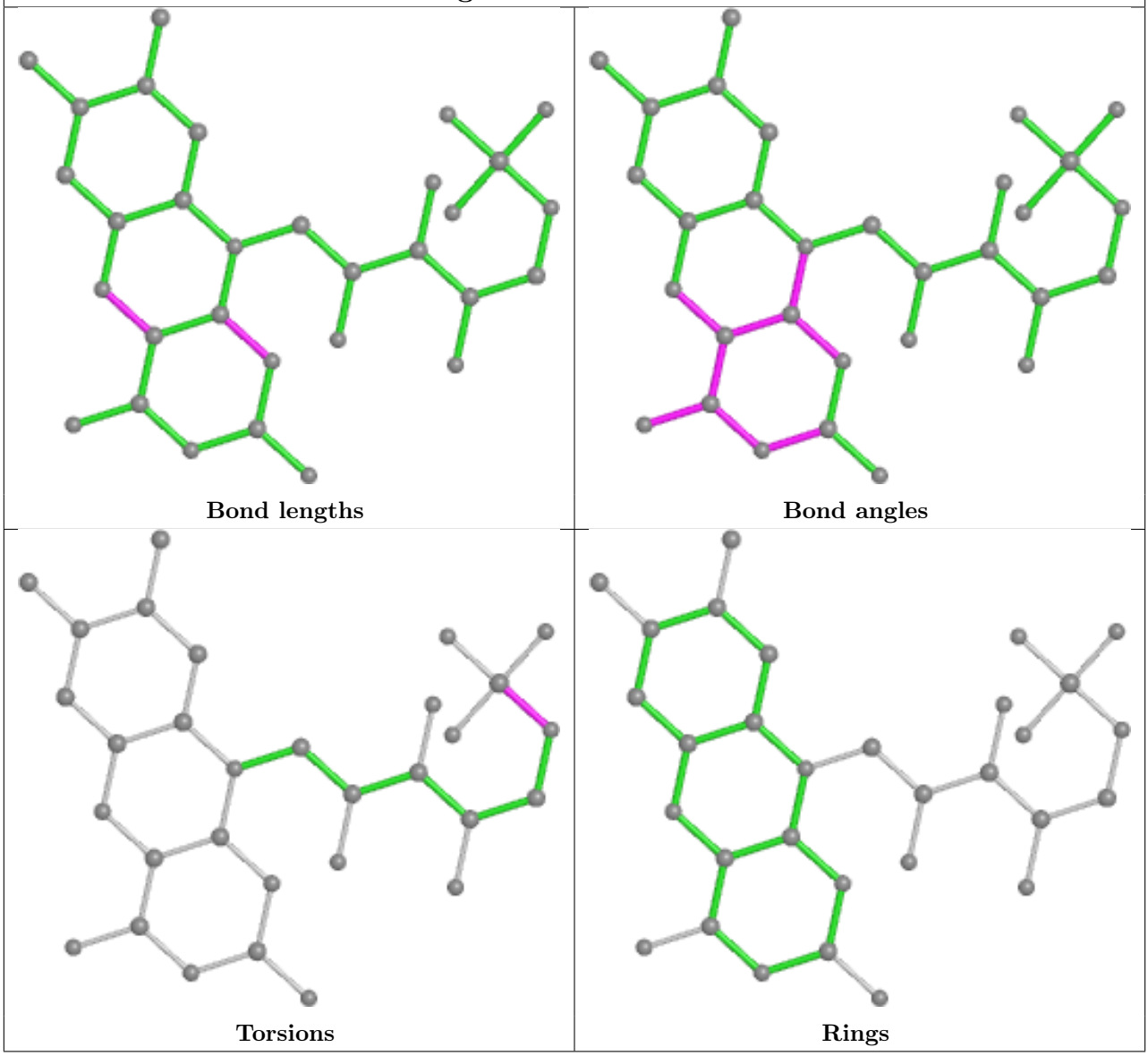


Torsions



Rings

Ligand FMN B 1002



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	374/415 (90%)	0.30	15 (4%) 38 28	17, 49, 93, 146	0
1	B	373/415 (89%)	0.53	33 (8%) 10 5	21, 61, 105, 133	0
All	All	747/830 (90%)	0.42	48 (6%) 19 12	17, 55, 99, 146	0

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	437	GLU	6.2
1	B	353	ASP	4.7
1	B	464	ASN	4.0
1	A	470	GLU	3.9
1	B	497	ASN	3.3
1	A	464	ASN	3.3
1	A	473	LYS	3.0
1	A	467	LYS	2.9
1	B	376	LYS	2.9
1	B	441	GLU	2.8
1	B	450	ASN	2.8
1	B	207	TYR	2.8
1	B	178	TYR	2.7
1	B	471	ASN	2.6
1	B	560	GLU	2.6
1	A	346	PRO	2.6
1	B	556	TYR	2.5
1	A	383	GLU	2.5
1	B	548	HIS	2.5
1	B	383	GLU	2.5
1	B	174	PHE	2.5
1	A	174	PHE	2.4
1	B	377	ASN	2.4
1	B	355	GLN	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	551	TYR	2.4
1	B	495	TYR	2.4
1	B	356	GLU	2.4
1	B	330	ASN	2.3
1	B	166	PHE	2.3
1	A	343	VAL	2.3
1	B	214	HIS	2.3
1	A	463	ILE	2.3
1	B	552	GLN	2.3
1	A	499	GLN	2.3
1	B	268	GLU	2.2
1	B	451	ILE	2.2
1	B	162	ASN	2.2
1	B	437	GLU	2.2
1	A	512	LEU	2.2
1	B	414	PHE	2.2
1	B	440	LYS	2.1
1	A	466	ILE	2.1
1	B	449	THR	2.1
1	B	442	ILE	2.1
1	A	441	GLU	2.1
1	A	414	PHE	2.1
1	B	564	ARG	2.1
1	B	444	ASP	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 (i)

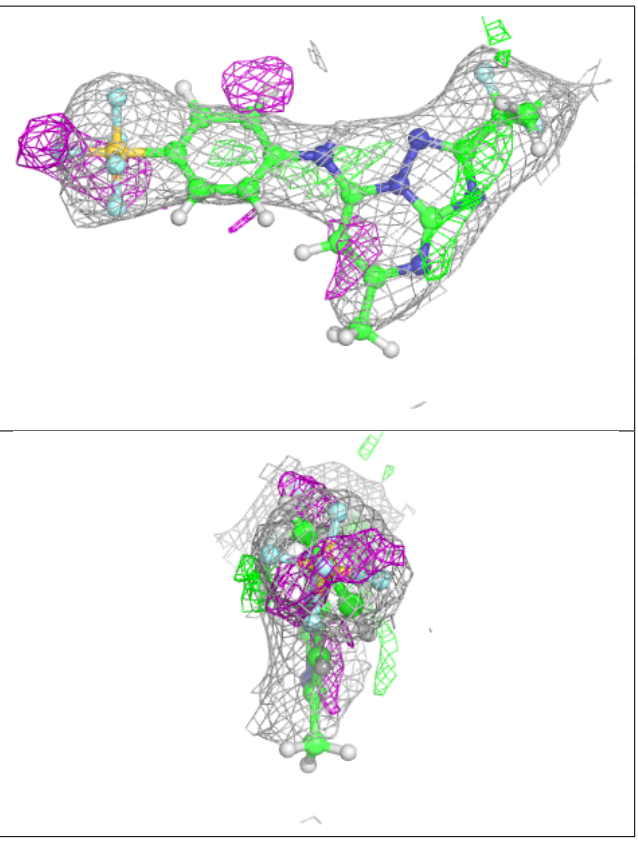
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	D65	A	1001	27/27	0.93	0.22	25,40,56,82	0
3	FMN	B	1002	31/31	0.94	0.19	5,16,30,37	0
2	D65	B	1001	27/27	0.95	0.20	11,22,63,78	0
4	ORO	A	1003	11/11	0.95	0.12	24,30,34,38	0
3	FMN	A	1002	31/31	0.96	0.14	9,18,27,35	0
4	ORO	B	1003	11/11	0.97	0.13	10,16,19,22	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.

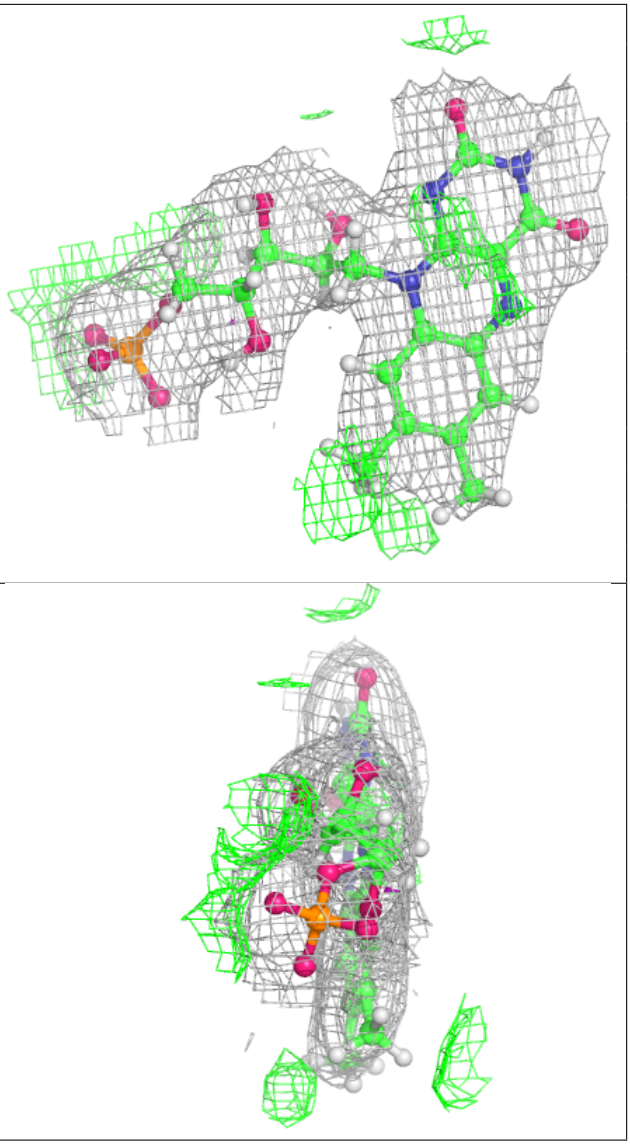
Electron density around D65 A 1001:

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 1002:

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



Electron density around D65 B 1001:

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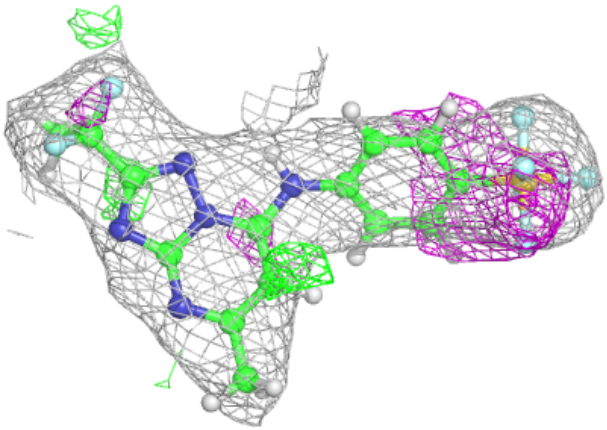
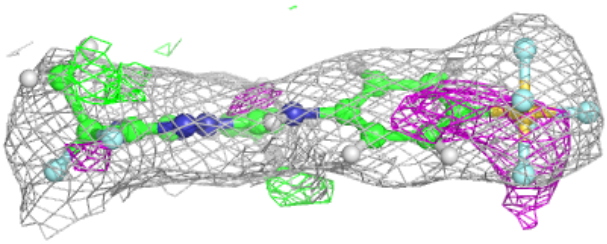
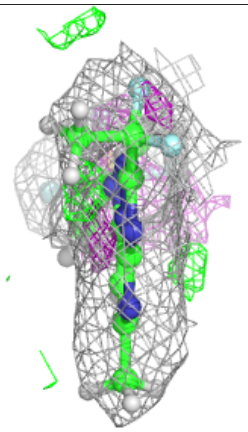
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

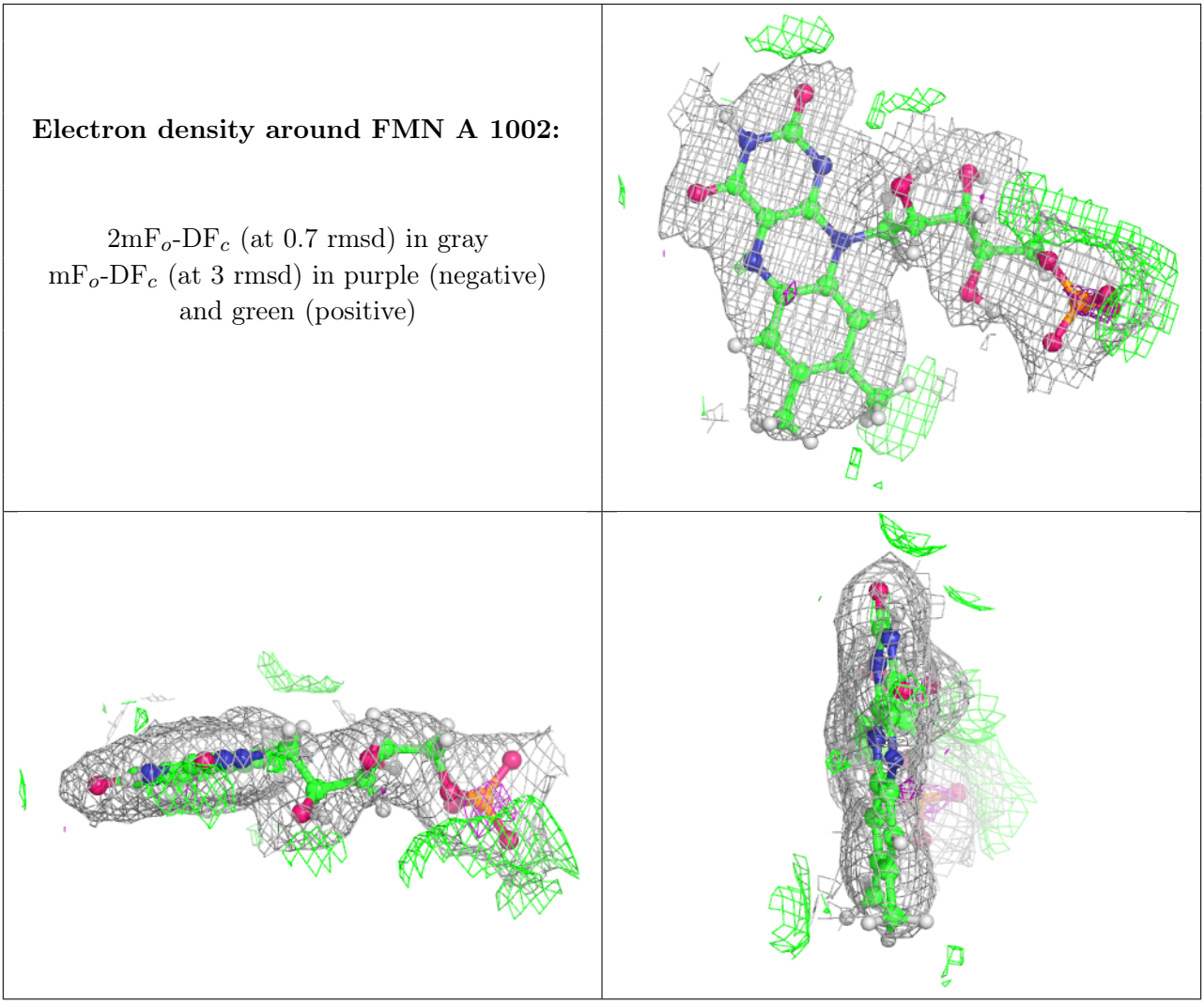






Electron density around FMN A 1002:

$2mF_o$-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.