Full wwPDB X-ray Structure Validation Report (i)

Feb 21, 2024 – 06:32 AM EST

PDB ID	:	4ORM
Title	:	Crystal structure of Plasmodium falciparum dihydroorotate dehydrogenase bound with Inhibitor DSM338 (N-[3,5-difluoro-4-(trifluoromethyl)phenyl]-5-methyl-2-(trifluoromethyl)[1,2,4]triazolo[1,5-a]pyrimidin-7-amine)
Authors	:	Deng, X.; Phillips, M.A.
Deposited on	:	2014-02-11
Resolution	:	2.07 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:

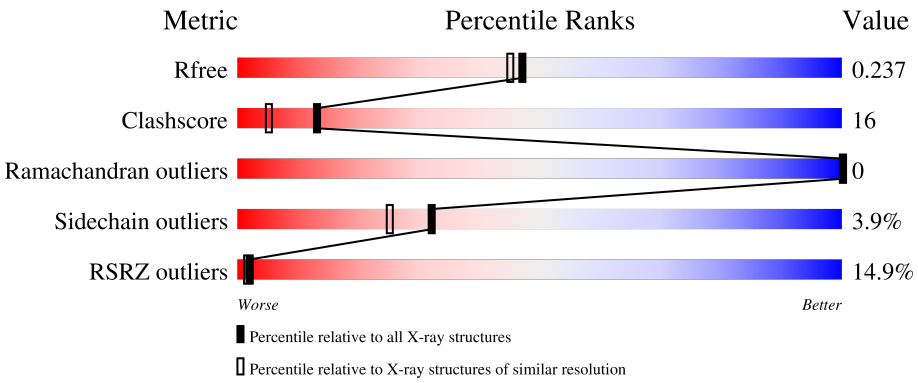
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.07 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	2684 (2.08-2.04)
Clashscore	141614	2801 (2.08-2.04)
Ramachandran outliers	138981	2768 (2.08-2.04)
Sidechain outliers	138945	2768 (2.08-2.04)
RSRZ outliers	127900	2646 (2.08-2.04)

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	401	14% 73% 19% • 6%

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 3194 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

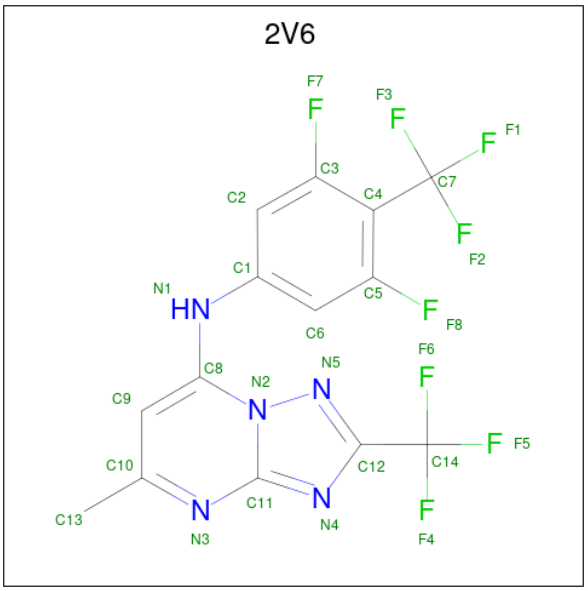
- Molecule 1 is a protein called Dihydroorotate dehydrogenase (quinone), mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	375	2992	1911	500	564	17	0	3	0

There are 19 discrepancies between the modelled and reference sequences:

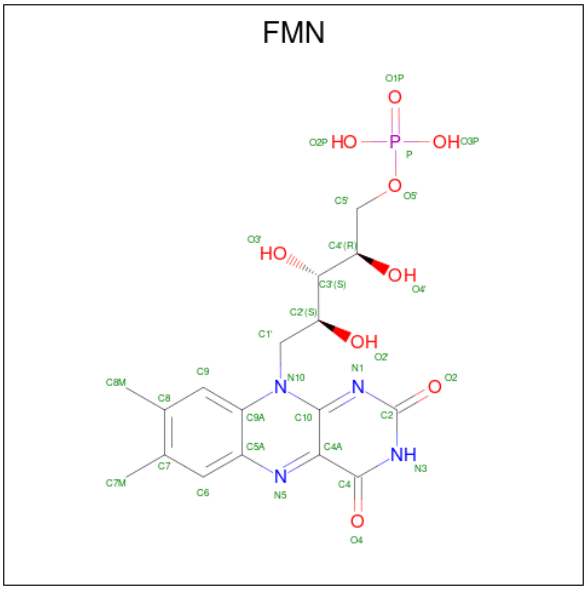
Chain	Residue	Modelled	Actual	Comment	Reference
A	139	MET	-	expression tag	UNP Q08210
A	140	GLY	-	expression tag	UNP Q08210
A	141	HIS	-	expression tag	UNP Q08210
A	142	HIS	-	expression tag	UNP Q08210
A	143	HIS	-	expression tag	UNP Q08210
A	144	HIS	-	expression tag	UNP Q08210
A	145	HIS	-	expression tag	UNP Q08210
A	146	HIS	-	expression tag	UNP Q08210
A	147	ALA	-	expression tag	UNP Q08210
A	148	GLU	-	expression tag	UNP Q08210
A	149	ASN	-	expression tag	UNP Q08210
A	150	LEU	-	expression tag	UNP Q08210
A	151	TYR	-	expression tag	UNP Q08210
A	152	PHE	-	expression tag	UNP Q08210
A	153	GLN	-	expression tag	UNP Q08210
A	154	GLY	-	expression tag	UNP Q08210
A	155	ALA	-	expression tag	UNP Q08210
A	156	ASP	-	expression tag	UNP Q08210
A	157	PRO	-	expression tag	UNP Q08210

- Molecule 2 is N-[3,5-difluoro-4-(trifluoromethyl)phenyl]-5-methyl-2-(trifluoromethyl)[1,2,4]triazolo[1,5-a]pyrimidin-7-amine (three-letter code: 2V6) (formula: $C_{14}H_7F_8N_5$).



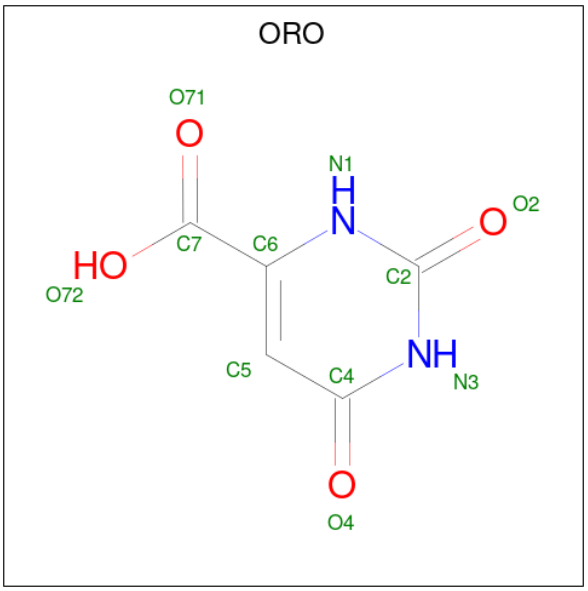
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	F	N		
2	A	1	27	14	8	5	0	0

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



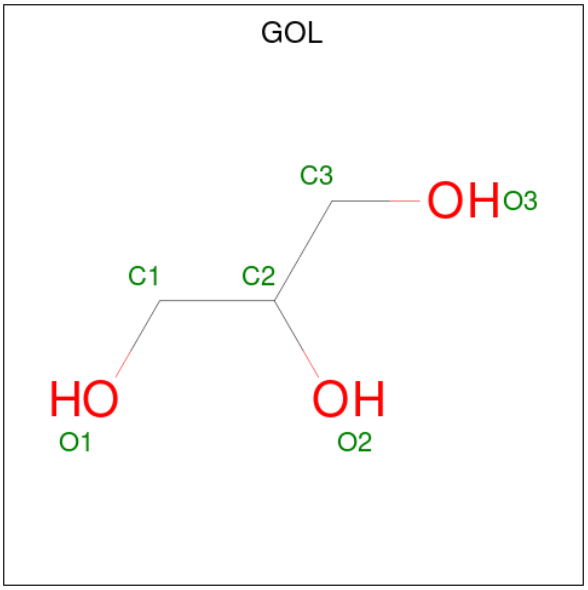
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
3	A	1	31	17	4	9	1	0	0

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



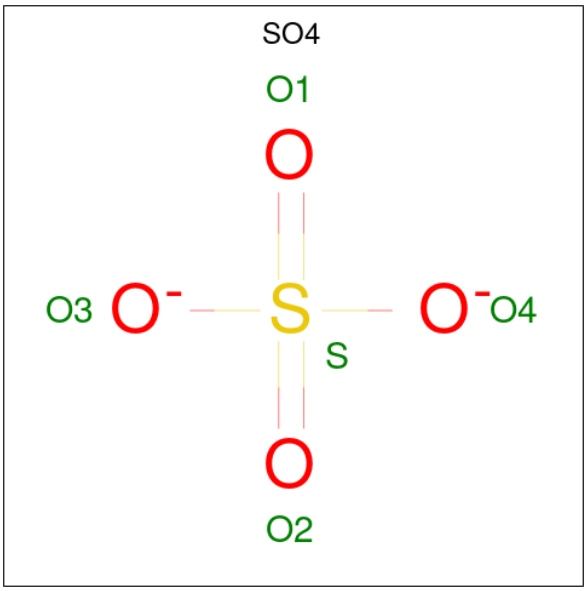
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
4	A	1	11	5	2	4	0	0

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



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

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total O S 5 4 1	0	0
6	A	1	Total O S 5 4 1	0	0

- Molecule 7 is water.

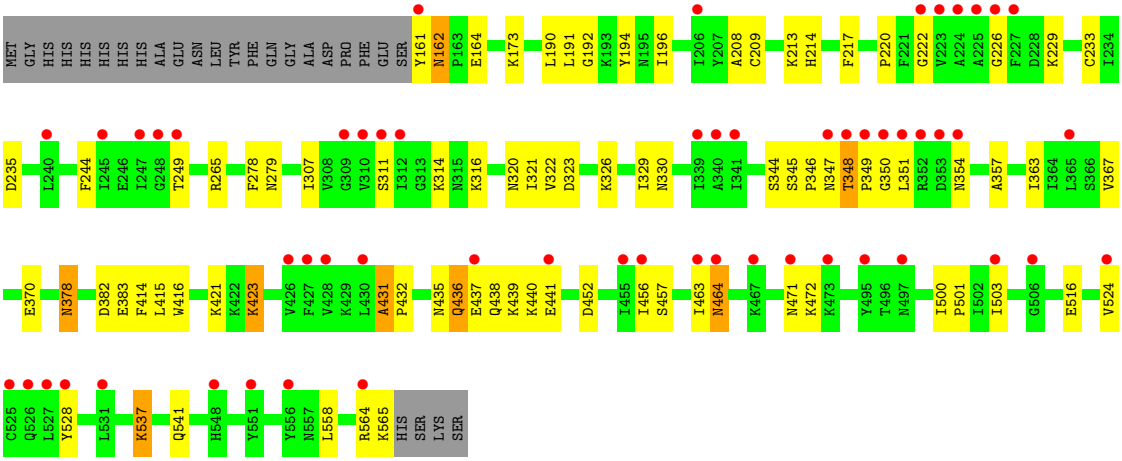
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	117	Total O 117 117	0	0

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:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 64	Depositor
Cell constants a, b, c, α, β, γ	85.47Å 85.47Å 138.28Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	28.00 – 2.07 27.98 – 2.03	Depositor EDS
% Data completeness (in resolution range)	99.0 (28.00-2.07) 99.0 (27.98-2.03)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$< I/\sigma(I) >$ [1]	2.35 (at 2.03Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.186 , 0.240 0.200 , 0.237	Depositor DCC
R_{free} test set	1832 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	44.3	Xtriage
Anisotropy	0.332	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 61.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.047 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	3194	wwPDB-VP
Average B, all atoms (Å^2)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.85% 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, GOL, SO4, FMN, 2V6

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	1.06	2/3042 (0.1%)	0.93	4/4096 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	349	PRO	N-CD	5.30	1.55	1.47
1	A	432	PRO	N-CD	5.12	1.55	1.47

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	500	ILE	C-N-CD	5.87	140.73	128.40
1	A	431	ALA	C-N-CD	5.67	140.31	128.40
1	A	162	ASN	C-N-CD	5.63	140.22	128.40
1	A	348	THR	C-N-CD	5.45	139.85	128.40

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	2992	0	3031	100	0
2	A	27	0	7	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	31	0	19	1	0
4	A	11	0	3	0	0
5	A	6	0	8	1	0
6	A	10	0	0	1	0
7	A	117	0	0	5	0
All	All	3194	0	3068	100	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 16.

All (100) 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:326:LYS:CD	1:A:370:GLU:HG3	1.86	1.04
1:A:321:ILE:HG21	1:A:354:ASN:HD21	1.25	1.02
1:A:326:LYS:HD2	1:A:370:GLU:HG3	1.03	1.01
1:A:326:LYS:HE3	1:A:370:GLU:HG2	1.44	0.97
1:A:326:LYS:HD2	1:A:370:GLU:CG	1.94	0.97
1:A:320:ASN:ND2	1:A:323:ASP:HB2	1.83	0.92
1:A:435:ASN:HD22	1:A:438:GLN:HG3	1.41	0.86
1:A:278:PHE:CD2	1:A:348:THR:HG23	2.10	0.86
1:A:278:PHE:CZ	1:A:345:SER:HB2	2.11	0.85
1:A:383:GLU:OE1	1:A:414:PHE:CZ	2.31	0.84
1:A:278:PHE:HD2	1:A:348:THR:HG23	1.44	0.82
1:A:320:ASN:HD22	1:A:323:ASP:HB2	1.43	0.81
1:A:278:PHE:CZ	1:A:345:SER:CB	2.65	0.80
1:A:321:ILE:HG13	1:A:322:VAL:H	1.45	0.80
1:A:321:ILE:CD1	1:A:363:ILE:HG12	2.11	0.80
1:A:278:PHE:HZ	1:A:345:SER:HB2	1.47	0.76
1:A:321:ILE:HG21	1:A:354:ASN:ND2	2.00	0.76
1:A:326:LYS:HE3	1:A:370:GLU:CG	2.16	0.76
1:A:191:LEU:HD22	1:A:196:ILE:HD11	1.70	0.74
1:A:346:PRO:HG2	1:A:347:ASN:CG	2.07	0.73
1:A:321:ILE:HG13	1:A:322:VAL:N	2.04	0.73
1:A:321:ILE:CG1	1:A:322:VAL:N	2.52	0.73
1:A:345:SER:OG	1:A:346:PRO:HD2	1.89	0.71
1:A:278:PHE:CD2	1:A:348:THR:CG2	2.75	0.70
1:A:321:ILE:HD11	1:A:322:VAL:HG23	1.73	0.69
1:A:217:PHE:CD1	1:A:307:ILE:HD12	2.29	0.67
1:A:435:ASN:O	1:A:439:LYS:HG3	1.92	0.67
1:A:383:GLU:OE1	1:A:414:PHE:CE1	2.47	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:357:ALA:HB2	1:A:441:GLU:HG3	1.77	0.67
1:A:326:LYS:CE	1:A:370:GLU:CG	2.73	0.66
1:A:346:PRO:HD2	1:A:347:ASN:H	1.59	0.66
1:A:321:ILE:HD12	1:A:322:VAL:N	2.10	0.65
1:A:321:ILE:HD11	1:A:363:ILE:HG12	1.78	0.65
1:A:346:PRO:CD	1:A:347:ASN:H	2.09	0.65
1:A:278:PHE:CE2	1:A:345:SER:CB	2.81	0.64
1:A:326:LYS:CD	1:A:370:GLU:CG	2.66	0.63
1:A:314:LYS:HG2	1:A:351:LEU:HD13	1.81	0.61
1:A:435:ASN:HD22	1:A:438:GLN:CG	2.10	0.61
1:A:278:PHE:HD2	1:A:348:THR:CG2	2.13	0.61
1:A:321:ILE:HD13	1:A:363:ILE:HG12	1.82	0.60
1:A:537:LYS:HD2	1:A:541:GLN:NE2	2.16	0.60
1:A:321:ILE:CD1	1:A:322:VAL:N	2.65	0.59
1:A:320:ASN:HB3	1:A:323:ASP:HB3	1.85	0.59
1:A:351:LEU:O	1:A:354:ASN:HB2	2.03	0.58
1:A:209[A]:CYS:SG	7:A:1185:HOH:O	2.57	0.57
1:A:278:PHE:HZ	1:A:345:SER:CB	2.11	0.57
1:A:164:GLU:OE2	6:A:1005:SO4:O2	2.23	0.56
1:A:346:PRO:CD	1:A:347:ASN:N	2.68	0.56
1:A:213:LYS:HB3	7:A:1134:HOH:O	2.05	0.56
1:A:322:VAL:O	1:A:326:LYS:HG2	2.06	0.56
1:A:321:ILE:HD11	1:A:363:ILE:CG1	2.36	0.55
1:A:435:ASN:HB2	1:A:438:GLN:HG3	1.90	0.54
1:A:357:ALA:HB2	1:A:441:GLU:CG	2.38	0.54
1:A:226:GLY:HA3	3:A:1002:FMN:N5	2.23	0.54
1:A:435:ASN:HB2	1:A:438:GLN:H	1.73	0.53
1:A:161:TYR:N	7:A:1178:HOH:O	2.42	0.52
1:A:471:ASN:CB	1:A:472:LYS:HD3	2.40	0.52
1:A:378:ASN:OD1	1:A:415:LEU:HD13	2.10	0.52
1:A:452:ASP:O	1:A:501:PRO:HD2	2.10	0.51
1:A:537:LYS:HD2	1:A:541:GLN:HE22	1.76	0.50
1:A:357:ALA:CB	1:A:441:GLU:HG3	2.42	0.50
1:A:321:ILE:CD1	1:A:363:ILE:CG1	2.87	0.50
1:A:346:PRO:HG2	1:A:347:ASN:ND2	2.26	0.49
1:A:278:PHE:CE2	1:A:345:SER:HB3	2.46	0.49
1:A:346:PRO:HG2	1:A:347:ASN:OD1	2.13	0.49
1:A:463:ILE:C	1:A:464:ASN:HD22	2.16	0.49
1:A:344:SER:HB2	1:A:431:ALA:HB2	1.93	0.49
1:A:350:GLY:O	1:A:351:LEU:HB3	2.13	0.49
1:A:516:GLU:OE1	7:A:1214:HOH:O	2.20	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:435:ASN:ND2	1:A:438:GLN:HG3	2.20	0.48
1:A:436:GLN:O	1:A:440:LYS:HG3	2.14	0.47
1:A:329:ILE:HD11	1:A:367:VAL:HG13	1.95	0.47
1:A:190:LEU:CD1	1:A:194:TYR:CE2	2.97	0.47
1:A:249:THR:HA	1:A:311:SER:HB3	1.95	0.47
1:A:321:ILE:HD12	1:A:322:VAL:CA	2.44	0.47
1:A:382:ASP:CG	5:A:1004:GOL:H32	2.36	0.47
1:A:416:TRP:CZ2	1:A:423:LYS:HB3	2.51	0.46
1:A:190:LEU:HD11	1:A:194:TYR:CE2	2.50	0.46
1:A:278:PHE:CE2	1:A:348:THR:HG23	2.50	0.46
1:A:278:PHE:CZ	1:A:345:SER:HB3	2.49	0.46
1:A:321:ILE:CD1	1:A:322:VAL:HG23	2.44	0.45
1:A:378:ASN:HB2	7:A:1126:HOH:O	2.16	0.45
1:A:190:LEU:CD1	1:A:194:TYR:HE2	2.30	0.44
1:A:330:ASN:HD22	1:A:330:ASN:HA	1.61	0.44
1:A:314:LYS:CD	1:A:351:LEU:HD13	2.49	0.43
1:A:192:GLY:HA3	1:A:233:CYS:SG	2.58	0.43
1:A:314:LYS:HE3	1:A:351:LEU:HB2	2.00	0.43
1:A:314:LYS:CG	1:A:351:LEU:HD13	2.47	0.43
1:A:222:GLY:HA3	1:A:244:PHE:CE1	2.54	0.43
1:A:321:ILE:HD12	1:A:322:VAL:HA	2.00	0.42
1:A:421:LYS:HD2	1:A:421:LYS:HA	1.83	0.42
1:A:435:ASN:ND2	1:A:438:GLN:CD	2.73	0.42
1:A:456:ILE:HA	1:A:457:SER:HA	1.88	0.42
1:A:229:LYS:HD3	1:A:279:ASN:O	2.19	0.42
1:A:503:ILE:HG13	1:A:524:VAL:HG12	2.02	0.42
1:A:208:ALA:O	1:A:220:PRO:HD3	2.19	0.41
1:A:213:LYS:HB3	1:A:214:HIS:H	1.62	0.41
1:A:437:GLU:HA	1:A:440:LYS:HD2	2.02	0.41
1:A:471:ASN:HB3	1:A:472:LYS:HD3	2.02	0.41
1:A:558:LEU:HD23	1:A:558:LEU:C	2.42	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	376/401 (94%)	367 (98%)	9 (2%)	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	335/354 (95%)	322 (96%)	13 (4%)	32 25

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	162	ASN
1	A	173	LYS
1	A	235	ASP
1	A	265	ARG
1	A	316	LYS
1	A	378	ASN
1	A	423	LYS
1	A	436	GLN
1	A	464	ASN
1	A	528	TYR
1	A	537	LYS
1	A	564	ARG
1	A	565	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	195	ASN
1	A	320	ASN
1	A	330	ASN

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Mol	Chain	Res	Type
1	A	354	ASN
1	A	377	ASN
1	A	435	ASN
1	A	436	GLN
1	A	450	ASN
1	A	464	ASN
1	A	541	GLN
1	A	548	HIS

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	$\#\|Z\| > 2$
3	FMN	A	1002	-	33,33,33	1.60	7 (21%)	48,50,50	1.66	14 (29%)
5	GOL	A	1004	-	5,5,5	0.72	0	5,5,5	1.49	1 (20%)
6	SO4	A	1006	-	4,4,4	0.41	0	6,6,6	0.58	0
2	2V6	A	1001	-	24,29,29	1.61	5 (20%)	35,46,46	2.37	8 (22%)
6	SO4	A	1005	-	4,4,4	0.34	0	6,6,6	0.46	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	ORO	A	1003	-	9,11,11	1.27	1 (11%)	8,15,15	2.52	5 (62%)

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
3	FMN	A	1002	-	-	1/18/18/18	0/3/3/3
4	ORO	A	1003	-	-	4/4/4/4	0/1/1/1
2	2V6	A	1001	-	-	0/16/16/16	0/3/3/3
5	GOL	A	1004	-	-	3/4/4/4	-

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1001	2V6	C4-C5	4.02	1.44	1.39
3	A	1002	FMN	C9A-C5A	3.95	1.47	1.41
2	A	1001	2V6	C9-C10	2.97	1.44	1.38
3	A	1002	FMN	C4A-N5	2.74	1.36	1.30
3	A	1002	FMN	C2-N3	-2.67	1.32	1.39
3	A	1002	FMN	C8-C7	2.60	1.47	1.40
2	A	1001	2V6	C1-N1	-2.39	1.35	1.40
3	A	1002	FMN	C1'-C2'	2.34	1.56	1.52
3	A	1002	FMN	C4'-C3'	2.21	1.57	1.53
3	A	1002	FMN	P-O5'	2.13	1.67	1.60
4	A	1003	ORO	C4-N3	2.12	1.36	1.33
2	A	1001	2V6	C10-N3	2.12	1.37	1.33
2	A	1001	2V6	C13-C10	2.10	1.55	1.50

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1001	2V6	N1-C8-N2	8.27	127.66	114.69
2	A	1001	2V6	C9-C8-N1	-6.80	113.02	123.36
4	A	1003	ORO	C6-C5-C4	4.12	119.39	116.73
2	A	1001	2V6	C9-C10-N3	-3.90	117.94	122.57
3	A	1002	FMN	C5A-C9A-N10	3.17	121.22	117.95
3	A	1002	FMN	C9A-C5A-N5	-3.16	119.00	122.43
4	A	1003	ORO	O71-C7-C6	3.10	127.53	121.24
2	A	1001	2V6	C8-C9-C10	3.03	119.36	117.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1002	FMN	P-O5'-C5'	2.88	126.22	118.30
2	A	1001	2V6	C2-C1-C6	2.86	123.40	119.57
4	A	1003	ORO	C5-C4-N3	-2.84	120.76	124.08
3	A	1002	FMN	O2-C2-N1	-2.83	117.14	121.83
3	A	1002	FMN	C4A-C10-N10	2.79	120.56	116.48
2	A	1001	2V6	F5-C14-F6	2.72	115.69	105.72
3	A	1002	FMN	C4-C4A-N5	2.67	122.03	118.23
4	A	1003	ORO	C7-C6-N1	2.66	120.40	116.48
3	A	1002	FMN	C9A-N10-C10	-2.56	116.77	120.77
3	A	1002	FMN	O3'-C3'-C2'	2.54	114.94	108.81
3	A	1002	FMN	O3P-P-O2P	2.40	116.81	107.64
3	A	1002	FMN	C5A-N5-C4A	2.29	121.88	118.07
3	A	1002	FMN	C4A-C10-N1	-2.27	119.47	124.73
5	A	1004	GOL	O1-C1-C2	2.26	121.06	110.20
3	A	1002	FMN	O2'-C2'-C3'	2.26	114.60	109.10
4	A	1003	ORO	C5-C6-N1	-2.26	119.31	123.40
3	A	1002	FMN	O3'-C3'-C4'	-2.16	103.61	108.81
3	A	1002	FMN	C10-C4A-N5	-2.05	120.52	124.86
2	A	1001	2V6	C2-C1-N1	-2.03	113.44	120.32
2	A	1001	2V6	C3-C4-C5	2.02	119.58	115.92

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1003	ORO	C5-C6-C7-O72
5	A	1004	GOL	O1-C1-C2-C3
4	A	1003	ORO	N1-C6-C7-O72
4	A	1003	ORO	C5-C6-C7-O71
5	A	1004	GOL	O1-C1-C2-O2
5	A	1004	GOL	O2-C2-C3-O3
3	A	1002	FMN	C4'-C5'-O5'-P
4	A	1003	ORO	N1-C6-C7-O71

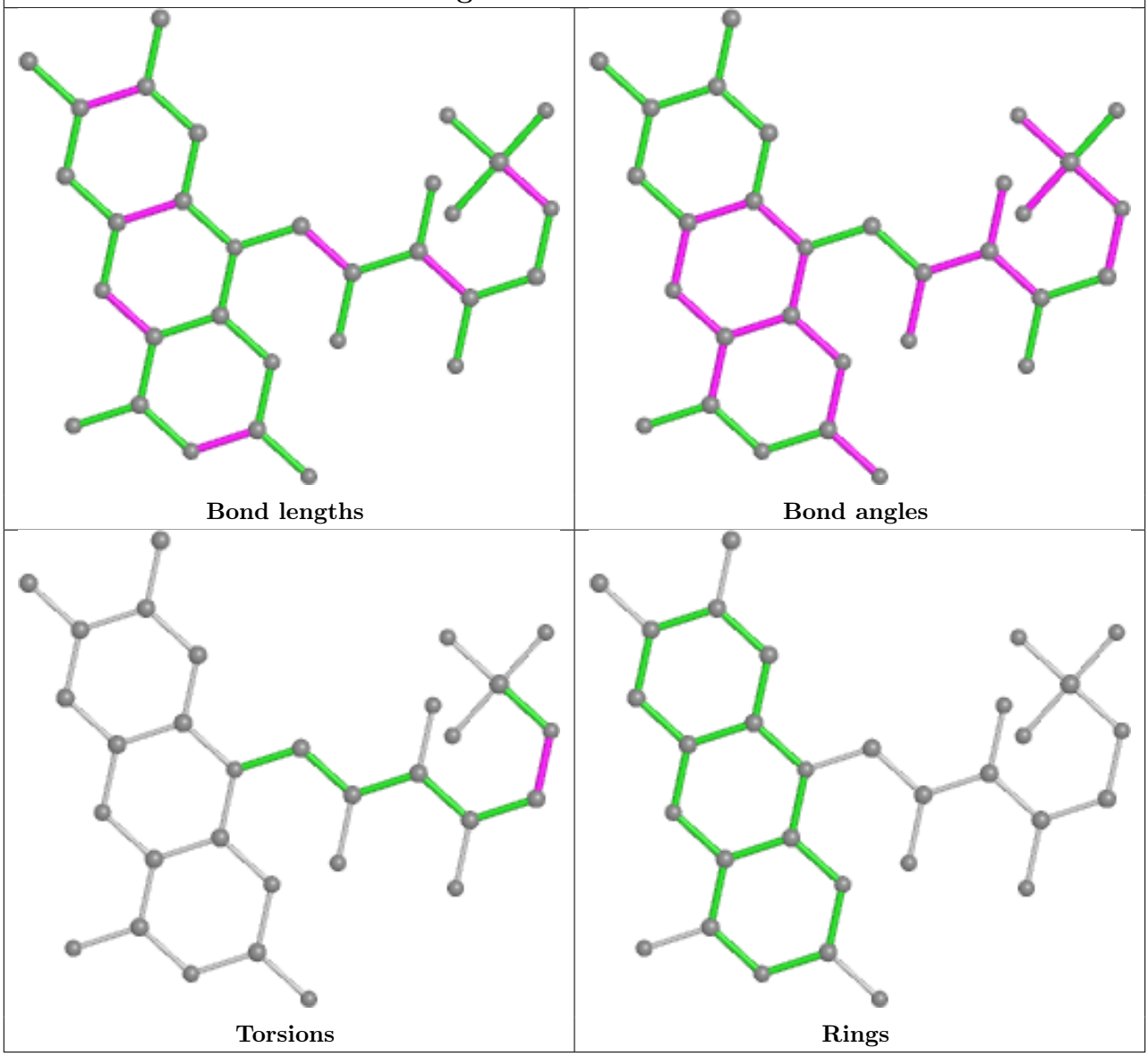
There are no ring outliers.

3 monomers are involved in 3 short contacts:

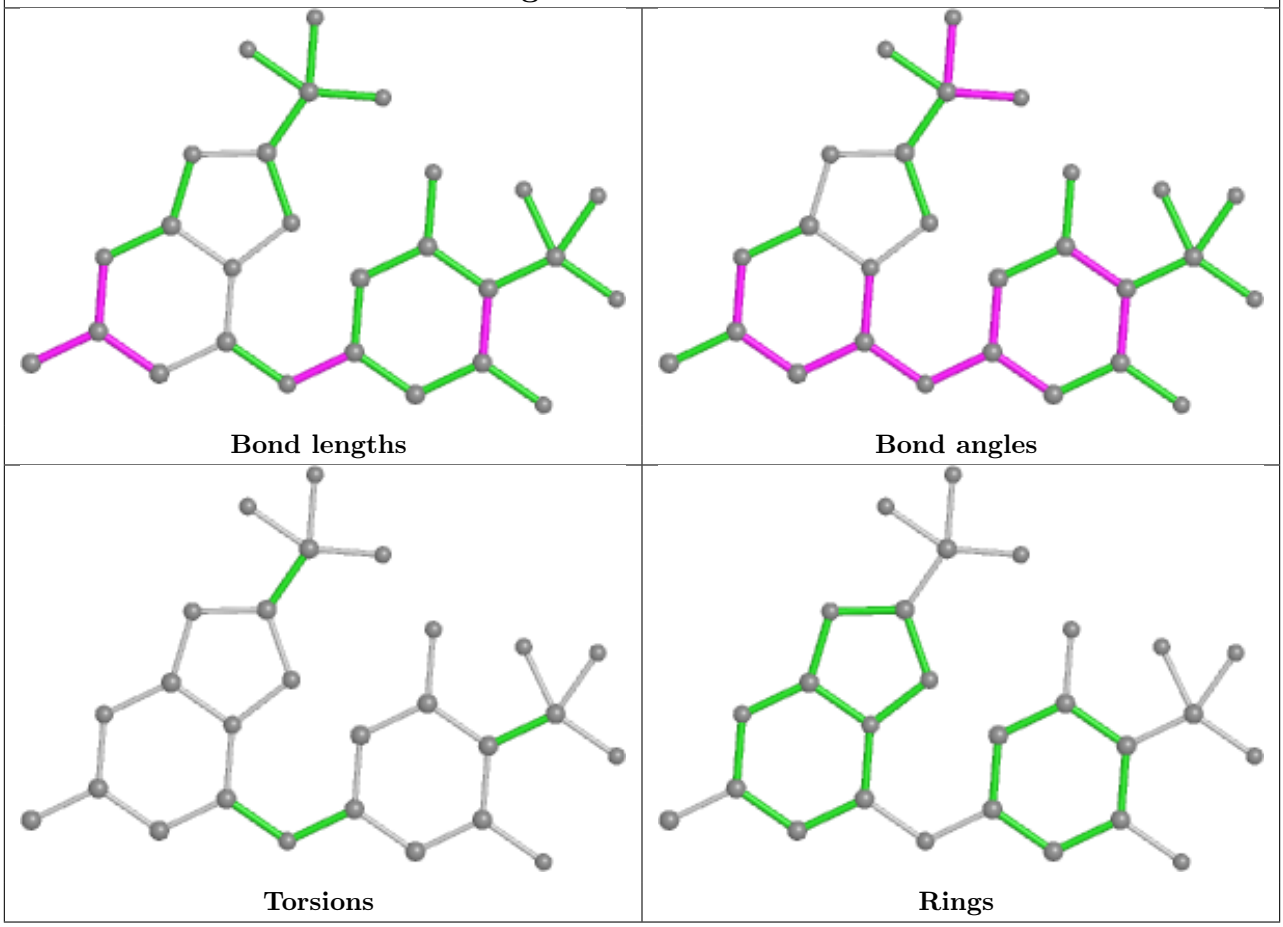
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1002	FMN	1	0
5	A	1004	GOL	1	0
6	A	1005	SO4	1	0

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 FMN A 1002



Ligand 2V6 A 1001



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	375/401 (93%)	0.63	56 (14%) 2 1	30, 50, 86, 113	0

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	161	TYR	7.4
1	A	349	PRO	5.7
1	A	556	TYR	5.2
1	A	441	GLU	5.0
1	A	353	ASP	4.8
1	A	455	ILE	4.6
1	A	467	LYS	4.4
1	A	350	GLY	4.3
1	A	564	ARG	4.2
1	A	223	VAL	4.1
1	A	341	ILE	4.0
1	A	351	LEU	3.9
1	A	310	VAL	3.9
1	A	224	ALA	3.9
1	A	473	LYS	3.7
1	A	471	ASN	3.7
1	A	551	TYR	3.6
1	A	352	ARG	3.5
1	A	354	ASN	3.5
1	A	464	ASN	3.4
1	A	348	THR	3.4
1	A	245	ILE	3.2
1	A	463	ILE	3.1
1	A	227	PHE	3.0
1	A	225	ALA	2.9
1	A	249	THR	2.9
1	A	527	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	528	TYR	2.8
1	A	309	GLY	2.8
1	A	339	ILE	2.7
1	A	427	PHE	2.7
1	A	206	ILE	2.7
1	A	311	SER	2.6
1	A	340	ALA	2.6
1	A	503	ILE	2.5
1	A	312	ILE	2.5
1	A	525	CYS	2.4
1	A	531	LEU	2.4
1	A	524	VAL	2.4
1	A	226	GLY	2.4
1	A	365	LEU	2.3
1	A	506	GLY	2.3
1	A	526	GLN	2.3
1	A	456	ILE	2.3
1	A	437	GLU	2.3
1	A	347	ASN	2.2
1	A	240	LEU	2.2
1	A	430	LEU	2.1
1	A	497	ASN	2.1
1	A	247	ILE	2.1
1	A	428	VAL	2.1
1	A	426	VAL	2.1
1	A	495	TYR	2.0
1	A	548	HIS	2.0
1	A	222	GLY	2.0
1	A	248	GLY	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)

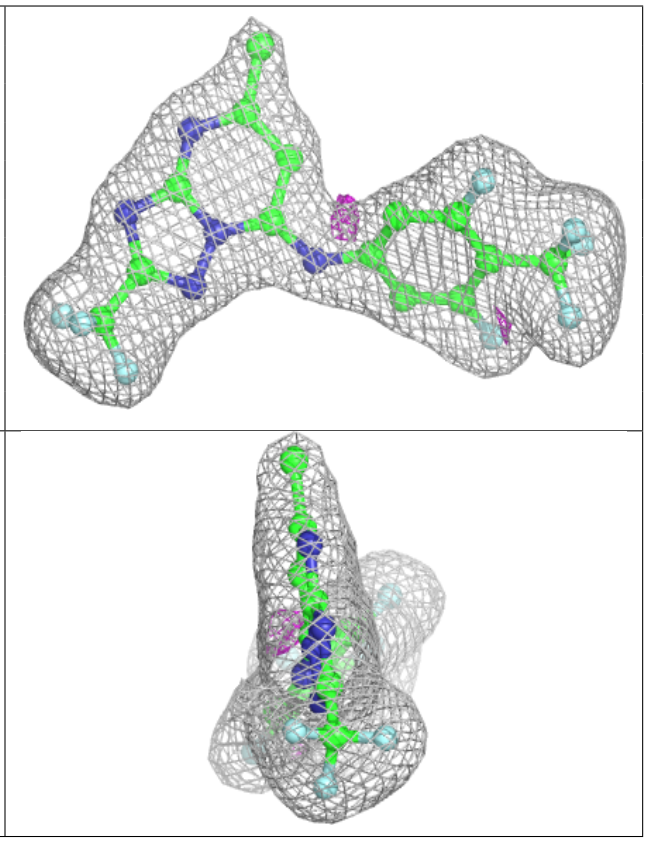
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	SO4	A	1006	5/5	0.83	0.39	30,30,30,30	0
6	SO4	A	1005	5/5	0.94	0.26	30,30,30,30	0
5	GOL	A	1004	6/6	0.95	0.11	46,48,53,53	0
2	2V6	A	1001	27/27	0.97	0.14	30,40,46,46	0
3	FMN	A	1002	31/31	0.97	0.23	33,38,42,44	0
4	ORO	A	1003	11/11	0.97	0.15	39,41,45,46	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.

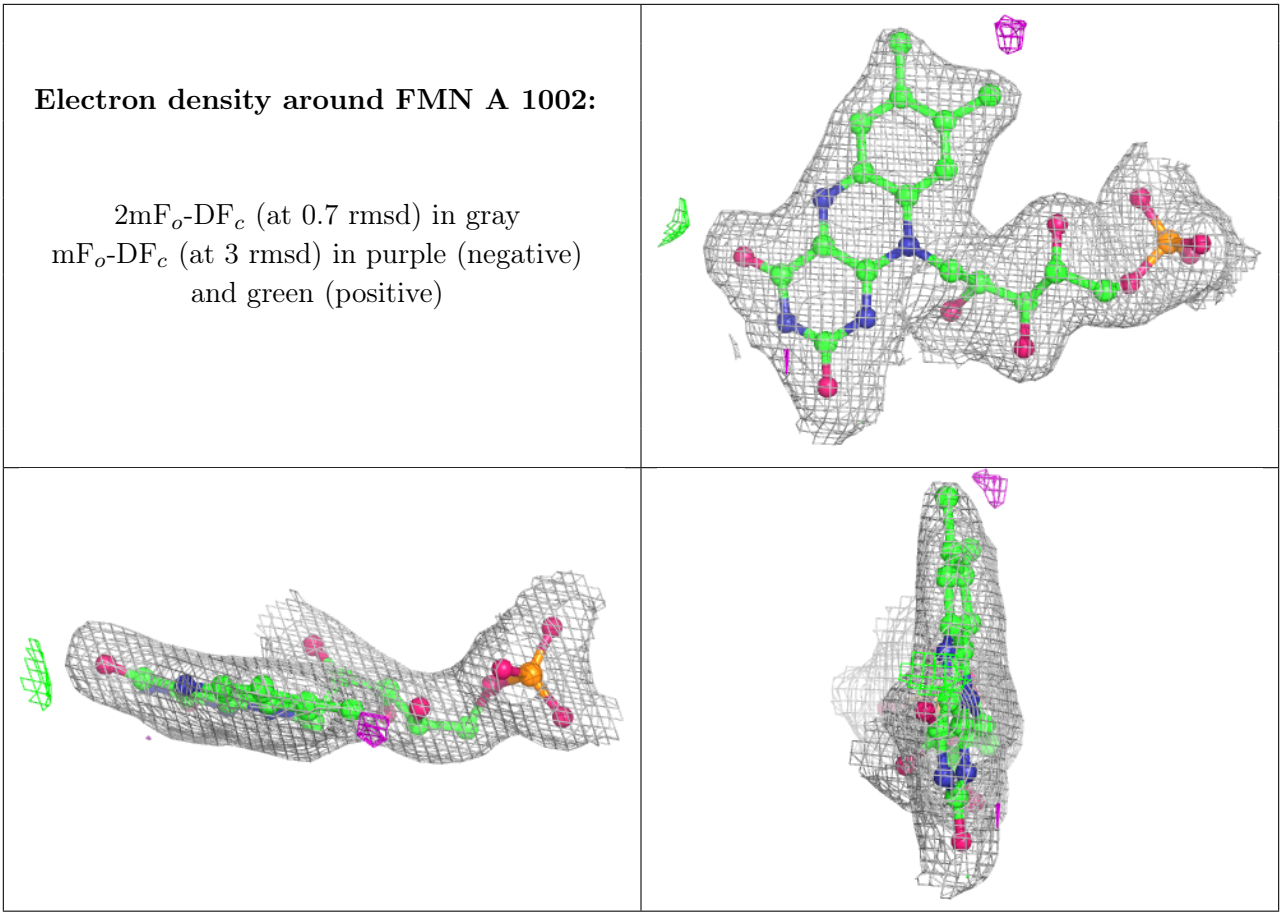
Electron density around 2V6 A 1001:

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 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.