Full wwPDB X-ray Structure Validation Report (i)

Aug 4, 2026 – 09:16 PM EDT

PDB ID	:	3W22 / pdb_00003w22
Title	:	Structure of Trypanosoma cruzi dihydroorotate dehydrogenase in complex with MII-3-125
Authors	:	Inaoka, D.K.; Iida, M.; Tabuchi, T.; Lee, N.; Matsuoka, S.; Shiba, T.; Sakamoto, K.; Suzuki, S.; Balogun, E.O.; Nara, T.; Aoki, T.; Inoue, M.; Honma, T.; Tanaka, A.; Harada, S.; Kita, K.
Deposited on	:	2012-11-26
Resolution	:	1.98 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:

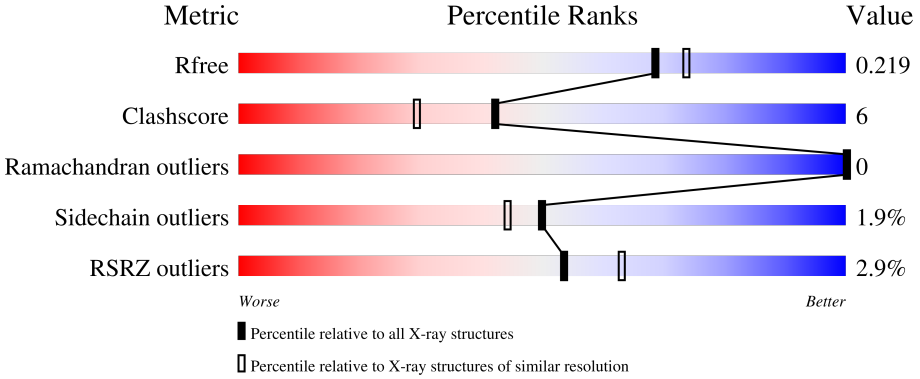
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

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 1.98 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1506 (1.98-1.98)
Clashscore	190562	1534 (1.98-1.98)
Ramachandran outliers	187476	1518 (1.98-1.98)
Sidechain outliers	187428	1518 (1.98-1.98)
RSRZ outliers	180081	1506 (1.98-1.98)

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	313	2% 84% 14% •
1	B	313	4% 85% 13% •

2 Entry composition (i)

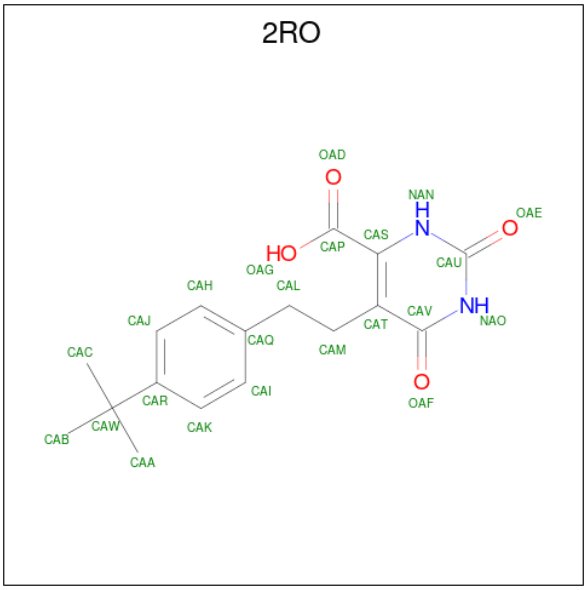
There are 6 unique types of molecules in this entry. The entry contains 5339 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 (fumarate).

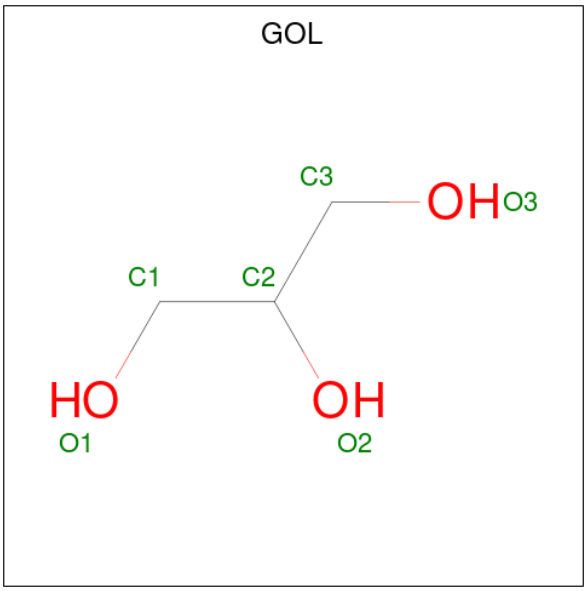
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	313	2388	1530	396	444	18	0	0	0
1	B	313	2388	1530	396	444	18	0	0	0

- Molecule 2 is 5-[2-(4-tert-butylphenyl)ethyl]-2,6-dioxo-1,2,3,6-tetrahydropyrimidine-4-carboxylic acid (CCD ID: 2RO) (formula: $C_{17}H_{20}N_2O_4$).



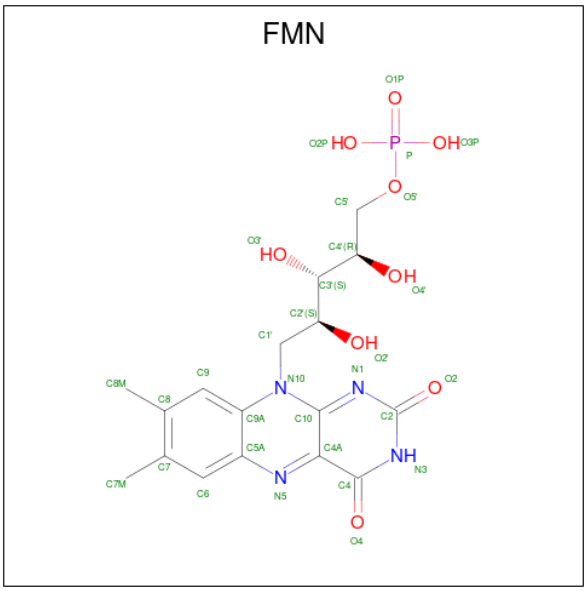
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	23	17	2	4	0	0
2	B	1	23	17	2	4	0	0

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



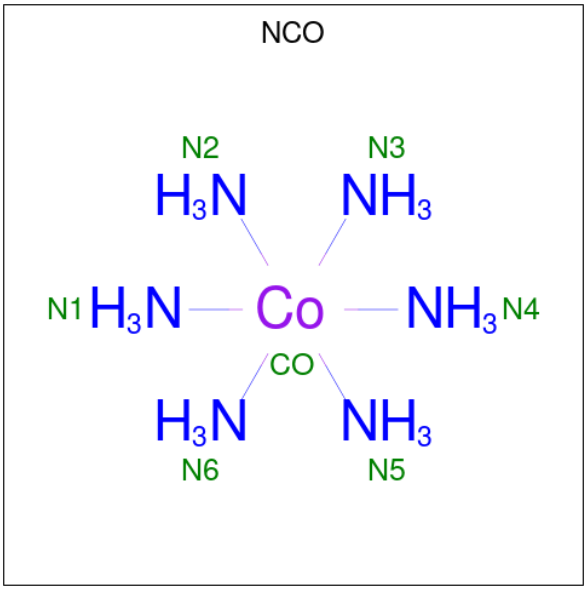
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
3	A	1	6	3	3	0	0
			Total	C	O		
3	A	1	6	3	3	0	0
			Total	C	O		
3	A	1	6	3	3	0	0
			Total	C	O		
3	A	1	6	3	3	0	0
			Total	C	O		
3	A	1	6	3	3	0	0
			Total	C	O		
3	B	1	6	3	3	0	0

- Molecule 4 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $C_{17}H_{21}N_4O_9P$).



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

- Molecule 5 is COBALT HEXAMMINE(III) (CCD ID: NCO) (formula: $CoH_{18}N_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	Co	N	0	0
			7	1	6		

- Molecule 6 is water.

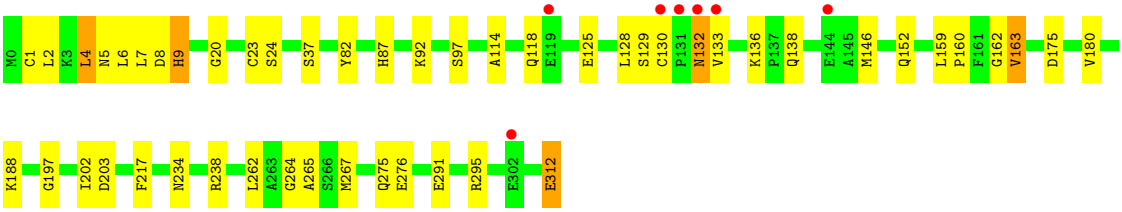
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	213	213	213	0	0
			Total	O		
6	B	199	199	199	0	0

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.

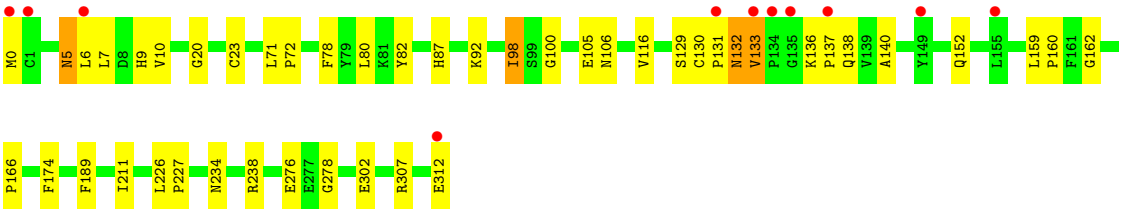
• Molecule 1: Dihydroorotate dehydrogenase (fumarate)

Chain A:



• Molecule 1: Dihydroorotate dehydrogenase (fumarate)

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	68.06Å 71.64Å 129.29Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.99 – 1.98 47.99 – 1.98	Depositor EDS
% Data completeness (in resolution range)	95.4 (47.99-1.98) 95.6 (47.99-1.98)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.03 (at 1.98Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.164 , 0.211 0.175 , 0.219	Depositor DCC
R_{free} test set	2274 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	22.1	Xtriage
Anisotropy	0.186	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 41.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.000 for k,h,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	5339	wwPDB-VP
Average B, all atoms (Å^2)	24.0	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 34.19 % 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 7.1007e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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: FMN, GOL, 2RO, NCO

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	1.39	17/2440 (0.7%)	1.11	1/3305 (0.0%)
1	B	1.30	8/2440 (0.3%)	1.15	8/3305 (0.2%)
All	All	1.34	25/4880 (0.5%)	1.13	9/6610 (0.1%)

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	276	GLU	C-O	-6.88	1.15	1.24
1	A	9	HIS	C-O	-6.55	1.15	1.23
1	A	1	CYS	C-O	-6.42	1.16	1.24
1	A	175	ASP	C-O	-6.36	1.16	1.24
1	A	163	VAL	N-CA	-6.24	1.38	1.46
1	A	23	CYS	C-O	-6.14	1.17	1.24
1	A	162	GLY	N-CA	6.07	1.50	1.45
1	A	2	LEU	C-O	-5.86	1.15	1.23
1	A	202	ILE	C-O	-5.83	1.17	1.24
1	A	24	SER	C-O	-5.83	1.16	1.24
1	B	23	CYS	N-CA	-5.63	1.41	1.46
1	A	203	ASP	C-O	-5.54	1.17	1.24
1	B	5	ASN	CA-C	-5.52	1.45	1.52
1	A	4	LEU	C-O	-5.39	1.17	1.23
1	A	265	ALA	C-O	-5.36	1.17	1.23
1	B	5	ASN	N-CA	-5.34	1.39	1.46
1	B	276	GLU	C-O	-5.31	1.17	1.24
1	B	131	PRO	N-CD	5.29	1.55	1.47
1	A	37	SER	N-CA	5.25	1.52	1.46
1	B	211	ILE	N-CA	-5.24	1.40	1.46
1	A	5	ASN	C-O	-5.21	1.18	1.24
1	B	130	CYS	C-N	5.20	1.40	1.33
1	B	174	PHE	C-O	-5.06	1.18	1.24
1	A	264	GLY	C-O	-5.04	1.18	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	267	MET	C-O	-5.01	1.17	1.23

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	278	GLY	CA-C-N	5.88	125.50	119.56
1	B	278	GLY	C-N-CA	5.88	125.50	119.56
1	A	197	GLY	N-CA-C	5.62	117.94	111.36
1	B	133	VAL	CA-C-N	-5.24	114.38	119.78
1	B	133	VAL	C-N-CA	-5.24	114.38	119.78
1	B	130	CYS	CA-C-N	-5.12	114.64	119.76
1	B	130	CYS	C-N-CA	-5.12	114.64	119.76
1	B	132	ASN	CA-C-N	5.08	131.53	122.13
1	B	132	ASN	C-N-CA	5.08	131.53	122.13

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	2388	0	2391	29	0
1	B	2388	0	2391	33	0
2	A	23	0	19	0	0
2	B	23	0	19	1	0
3	A	30	0	40	1	0
3	B	6	0	8	0	0
4	A	31	0	19	1	0
4	B	31	0	19	1	0
5	A	7	0	0	0	0
6	A	213	0	0	1	0
6	B	199	0	0	1	0
All	All	5339	0	4906	62	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 6.

All (62) 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:133:VAL:CG2	1:B:136:LYS:HG3	2.02	0.89
1:B:132:ASN:O	1:B:133:VAL:HG13	1.79	0.83
1:B:98:ILE:CD1	1:B:106:ASN:OD1	2.34	0.76
1:B:98:ILE:HD12	1:B:106:ASN:OD1	1.90	0.71
1:B:133:VAL:CG2	1:B:136:LYS:HE2	2.22	0.69
1:A:132:ASN:HD22	1:A:133:VAL:H	1.42	0.68
1:B:132:ASN:C	1:B:133:VAL:HG13	2.20	0.66
1:B:234:ASN:HD21	1:B:238:ARG:HE	1.44	0.64
1:B:133:VAL:HG21	1:B:136:LYS:HE2	1.79	0.64
1:A:114:ALA:O	1:A:118:GLN:HG3	1.98	0.63
1:B:132:ASN:O	1:B:133:VAL:CG1	2.47	0.62
1:B:82:TYR:OH	1:B:87:HIS:HD2	1.83	0.60
1:B:20:GLY:HA3	4:B:403:FMN:N5	2.17	0.58
1:A:6:LEU:HD12	1:A:6:LEU:C	2.30	0.56
1:A:128:LEU:HD12	1:A:163:VAL:HG11	1.87	0.56
1:B:7:LEU:O	1:B:9:HIS:HD2	1.88	0.56
1:B:71:LEU:HD22	2:B:401:2RO:CAH	2.36	0.56
1:A:160:PRO:HB3	1:A:188:LYS:HG3	1.89	0.54
1:B:133:VAL:HG21	1:B:136:LYS:HG3	1.89	0.54
1:B:133:VAL:HG22	1:B:136:LYS:HE2	1.90	0.54
1:A:234:ASN:HD21	1:A:238:ARG:HE	1.55	0.54
1:A:217:PHE:CE1	3:A:404:GOL:H12	2.44	0.53
1:A:7:LEU:O	1:A:9:HIS:HD2	1.92	0.52
1:B:234:ASN:ND2	1:B:238:ARG:HE	2.07	0.52
1:B:307:ARG:NH2	6:B:565:HOH:O	2.42	0.51
1:B:140:ALA:HB3	1:B:166:PRO:HG3	1.93	0.50
1:B:132:ASN:HB2	1:B:137:PRO:O	2.11	0.50
1:A:118:GLN:CG	1:A:159:LEU:HD11	2.41	0.49
1:A:128:LEU:HD12	1:A:163:VAL:CG1	2.43	0.49
1:A:234:ASN:ND2	1:A:238:ARG:HE	2.11	0.49
1:A:20:GLY:HA3	4:A:407:FMN:N5	2.28	0.48
1:B:132:ASN:C	1:B:133:VAL:CG1	2.88	0.47
1:B:133:VAL:HG23	1:B:136:LYS:HG3	1.93	0.47
1:A:87:HIS:HE1	1:A:92:LYS:O	1.99	0.46
1:A:312:GLU:OE2	1:A:312:GLU:CA	2.63	0.46
1:A:82:TYR:OH	1:A:87:HIS:HD2	1.97	0.46
1:A:312:GLU:OE2	1:A:312:GLU:N	2.48	0.46
1:B:159:LEU:HB3	1:B:160:PRO:HD2	1.99	0.45
1:B:5:ASN:ND2	1:B:10:VAL:HG22	2.32	0.45
1:B:80:LEU:HD11	1:B:116:VAL:HG21	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:146:MET:HE2	1:A:180:VAL:HG11	2.00	0.44
1:B:87:HIS:HE1	1:B:92:LYS:O	2.00	0.44
1:A:275:GLN:NE2	6:A:594:HOH:O	2.34	0.44
1:B:129:SER:HA	1:B:138:GLN:NE2	2.32	0.44
1:B:162:GLY:HA3	1:B:189:PHE:CE1	2.52	0.44
1:A:7:LEU:O	1:A:9:HIS:CD2	2.70	0.43
1:A:129:SER:HA	1:A:138:GLN:NE2	2.33	0.43
1:B:133:VAL:HG22	1:B:136:LYS:HG3	1.96	0.43
1:B:226:LEU:HB3	1:B:227:PRO:HD3	2.00	0.43
1:A:118:GLN:HG2	1:A:159:LEU:HD11	2.01	0.42
1:A:129:SER:O	1:A:130:CYS:C	2.60	0.42
1:A:133:VAL:HG22	1:A:136:LYS:HD3	2.01	0.41
1:A:291:GLU:OE2	1:A:295:ARG:NH1	2.54	0.41
1:B:152:GLN:HE21	1:B:152:GLN:HB3	1.75	0.41
1:A:7:LEU:O	1:A:8:ASP:HB2	2.20	0.41
1:A:133:VAL:HG23	1:A:136:LYS:HG3	2.03	0.41
1:A:128:LEU:HG	1:A:163:VAL:HG13	2.03	0.41
1:A:128:LEU:CD1	1:A:163:VAL:HG11	2.51	0.41
1:B:71:LEU:N	1:B:72:PRO:CD	2.84	0.41
1:B:78:PHE:CD2	1:B:78:PHE:C	2.98	0.41
1:A:97:SER:HA	1:A:125:GLU:O	2.22	0.40
1:B:100:GLY:HA3	1:B:105:GLU:HG2	2.04	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	311/313 (99%)	301 (97%)	10 (3%)	0	100	100
1	B	311/313 (99%)	302 (97%)	9 (3%)	0	100	100
All	All	622/626 (99%)	603 (97%)	19 (3%)	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	258/258 (100%)	253 (98%)	5 (2%)	50	44
1	B	258/258 (100%)	253 (98%)	5 (2%)	50	44
All	All	516/516 (100%)	506 (98%)	10 (2%)	50	44

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LEU
1	A	132	ASN
1	A	152	GLN
1	A	262	LEU
1	A	312	GLU
1	B	0	MET
1	B	6	LEU
1	B	98	ILE
1	B	302	GLU
1	B	312	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	HIS
1	A	87	HIS
1	A	132	ASN
1	A	138	GLN
1	A	152	GLN
1	A	234	ASN
1	B	5	ASN
1	B	9	HIS
1	B	87	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	118	GLN
1	B	152	GLN
1	B	234	ASN
1	B	275	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

11 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	GOL	A	404	-	5,5,5	0.33	0	5,5,5	0.23	0
2	2RO	A	401	-	24,24,24	1.89	7 (29%)	33,35,35	1.81	8 (24%)
3	GOL	A	406	-	5,5,5	0.63	0	5,5,5	0.43	0
3	GOL	A	403	-	5,5,5	0.32	0	5,5,5	0.88	0
3	GOL	B	402	-	5,5,5	0.67	0	5,5,5	0.75	0
3	GOL	A	402	-	5,5,5	0.64	0	5,5,5	0.72	0
2	2RO	B	401	-	24,24,24	1.80	8 (33%)	33,35,35	2.08	7 (21%)
5	NCO	A	408	-	6,6,6	1.70	2 (33%)	-		
4	FMN	A	407	-	33,33,33	1.66	7 (21%)	48,50,50	1.45	7 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	GOL	A	405	-	5,5,5	0.56	0	5,5,5	0.84	0
4	FMN	B	403	-	33,33,33	1.95	9 (27%)	48,50,50	1.62	10 (20%)

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	GOL	A	404	-	-	0/4/4/4	-
2	2RO	A	401	-	-	4/15/15/15	0/2/2/2
3	GOL	A	406	-	-	0/4/4/4	-
3	GOL	A	403	-	-	0/4/4/4	-
3	GOL	B	402	-	-	4/4/4/4	-
3	GOL	A	402	-	-	2/4/4/4	-
2	2RO	B	401	-	-	5/15/15/15	0/2/2/2
4	FMN	A	407	-	-	4/18/18/18	0/3/3/3
3	GOL	A	405	-	-	1/4/4/4	-
4	FMN	B	403	-	-	1/18/18/18	0/3/3/3

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	403	FMN	C9A-C5A	5.56	1.50	1.41
2	A	401	2RO	CAM-CAT	-5.06	1.38	1.51
4	A	407	FMN	C9A-C5A	4.34	1.48	1.41
4	B	403	FMN	C4-N3	-3.76	1.31	1.38
4	B	403	FMN	C4A-N5	3.63	1.38	1.30
4	A	407	FMN	C8-C7	3.62	1.49	1.40
2	B	401	2RO	CAJ-CAH	3.48	1.44	1.38
2	B	401	2RO	OAD-CAP	3.29	1.30	1.22
4	A	407	FMN	C4-N3	-3.21	1.32	1.38
4	B	403	FMN	C8-C7	3.15	1.48	1.40
4	B	403	FMN	C5A-N5	-3.13	1.33	1.39
5	A	408	NCO	CO-N5	3.04	2.06	1.96
4	B	403	FMN	C9-C8	-3.04	1.35	1.39
4	B	403	FMN	C10-N10	2.91	1.43	1.37
4	A	407	FMN	C2-N3	-2.84	1.32	1.39
2	A	401	2RO	CAS-CAP	-2.83	1.44	1.48
4	B	403	FMN	O4-C4	2.80	1.28	1.23
2	A	401	2RO	CAW-CAR	-2.78	1.48	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	2RO	CAL-CAQ	-2.74	1.44	1.51
4	A	407	FMN	C6-C5A	2.50	1.43	1.40
4	A	407	FMN	C5'-C4'	2.49	1.55	1.51
2	B	401	2RO	CAS-CAP	-2.48	1.44	1.48
2	B	401	2RO	CAJ-CAR	2.32	1.43	1.39
5	A	408	NCO	CO-N6	2.31	2.04	1.96
2	B	401	2RO	CAU-NAO	2.30	1.41	1.37
4	B	403	FMN	C8M-C8	2.24	1.55	1.51
2	B	401	2RO	CAK-CAR	2.19	1.43	1.39
2	A	401	2RO	CAV-NAO	2.18	1.42	1.38
2	B	401	2RO	CAS-CAT	2.15	1.41	1.37
2	A	401	2RO	CAU-NAN	2.07	1.40	1.37
2	B	401	2RO	CAV-CAT	-2.04	1.41	1.44
4	A	407	FMN	P-O2P	-2.04	1.47	1.54
2	A	401	2RO	CAS-CAT	2.02	1.41	1.37

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	401	2RO	CAT-CAV-NAO	7.63	121.50	115.70
2	B	401	2RO	CAM-CAT-CAV	5.44	123.93	116.64
2	A	401	2RO	CAT-CAV-NAO	4.90	119.42	115.70
2	A	401	2RO	CAM-CAT-CAV	4.69	122.93	116.64
4	B	403	FMN	C5A-C9A-N10	3.80	121.40	117.97
4	B	403	FMN	C1'-N10-C9A	3.67	127.77	120.63
2	B	401	2RO	OAF-CAV-NAO	-3.66	113.22	120.11
2	B	401	2RO	CAV-NAO-CAU	-3.65	121.34	126.37
2	A	401	2RO	CAK-CAR-CAW	3.48	128.59	121.47
4	B	403	FMN	O4-C4-C4A	-3.32	117.76	126.53
4	B	403	FMN	O4-C4-N3	3.26	126.23	120.11
4	A	407	FMN	C9A-C5A-N5	-3.23	119.03	122.45
4	A	407	FMN	O2P-P-O1P	3.22	123.39	110.83
4	A	407	FMN	O2-C2-N1	-3.21	116.47	121.80
4	B	403	FMN	O2-C2-N1	-3.03	116.76	121.80
4	A	407	FMN	O3P-P-O5'	-3.03	98.78	106.67
2	A	401	2RO	CAV-NAO-CAU	-2.85	122.44	126.37
4	B	403	FMN	C8M-C8-C9	-2.83	114.59	119.57
4	B	403	FMN	O2P-P-O5'	-2.83	99.30	106.67
2	A	401	2RO	CAM-CAL-CAQ	-2.51	103.89	112.70
2	A	401	2RO	CAJ-CAR-CAW	-2.49	116.38	121.47
4	B	403	FMN	C8M-C8-C7	2.41	125.69	120.76
4	B	403	FMN	C9A-N10-C10	-2.33	117.20	120.75

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	401	2RO	CAK-CAI-CAQ	2.31	124.04	121.00
4	A	407	FMN	O4-C4-C4A	-2.31	120.43	126.53
2	B	401	2RO	CAB-CAW-CAR	2.27	115.71	110.35
4	A	407	FMN	C4-C4A-N5	2.25	121.31	118.21
2	B	401	2RO	CAI-CAQ-CAH	-2.21	114.95	118.23
4	A	407	FMN	C5A-N5-C4A	2.15	121.57	118.09
2	A	401	2RO	CAK-CAR-CAJ	-2.11	114.89	118.03
4	B	403	FMN	O3P-P-O1P	2.06	118.85	110.83
2	A	401	2RO	OAF-CAV-NAO	-2.01	116.34	120.11

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	2RO	OAG-CAP-CAS-NAN
2	A	401	2RO	CAQ-CAL-CAM-CAT
2	B	401	2RO	OAG-CAP-CAS-NAN
2	B	401	2RO	CAQ-CAL-CAM-CAT
3	B	402	GOL	O1-C1-C2-C3
3	B	402	GOL	C1-C2-C3-O3
3	A	402	GOL	C1-C2-C3-O3
3	A	405	GOL	O1-C1-C2-C3
3	A	402	GOL	O2-C2-C3-O3
3	B	402	GOL	O1-C1-C2-O2
3	B	402	GOL	O2-C2-C3-O3
4	B	403	FMN	C4'-C5'-O5'-P
2	A	401	2RO	OAD-CAP-CAS-NAN
4	A	407	FMN	O3'-C3'-C4'-C5'
4	A	407	FMN	C4'-C5'-O5'-P
2	B	401	2RO	CAL-CAM-CAT-CAV
4	A	407	FMN	C2'-C3'-C4'-O4'
4	A	407	FMN	O3'-C3'-C4'-O4'
2	A	401	2RO	OAG-CAP-CAS-CAT
2	B	401	2RO	OAD-CAP-CAS-CAT
2	B	401	2RO	OAD-CAP-CAS-NAN

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	404	GOL	1	0

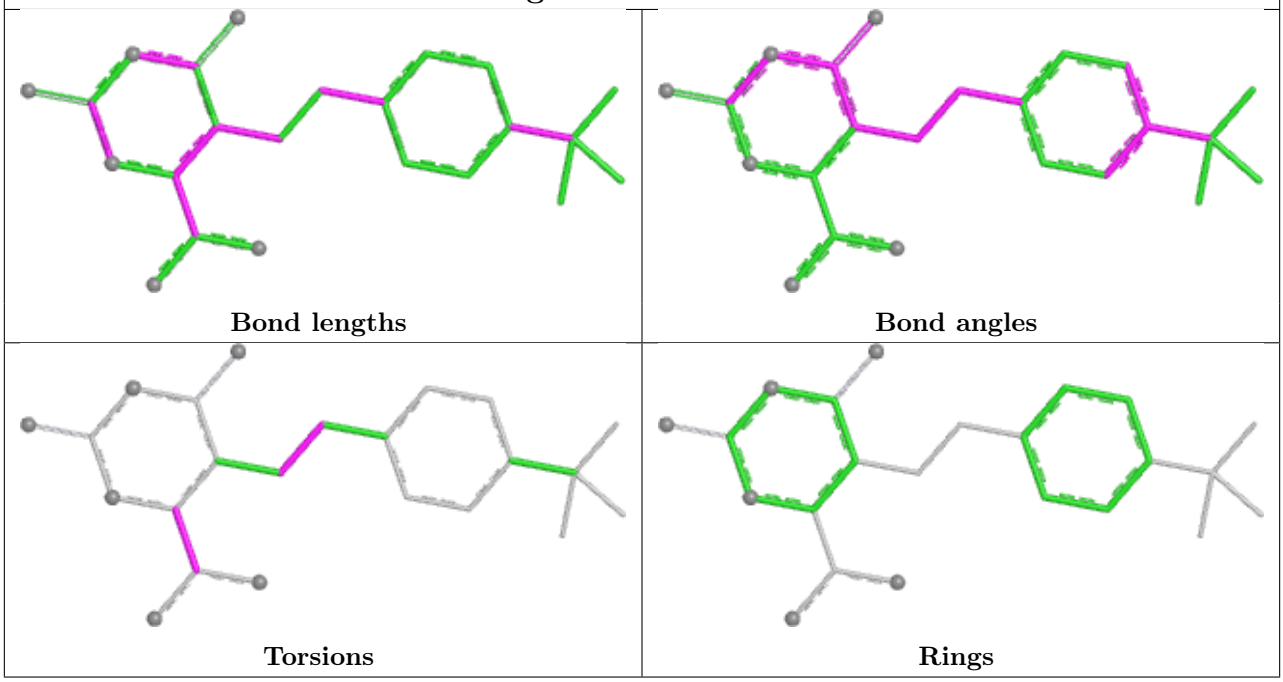
Continued on next page...

Continued from previous page...

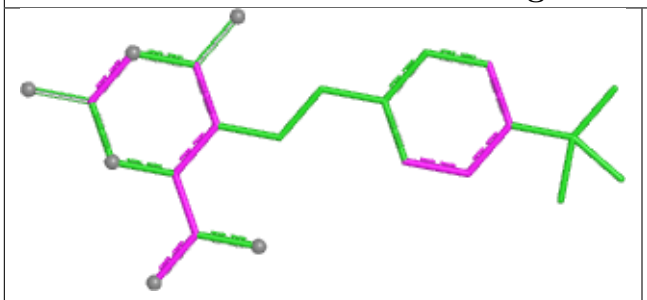
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	401	2RO	1	0
4	A	407	FMN	1	0
4	B	403	FMN	1	0

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.

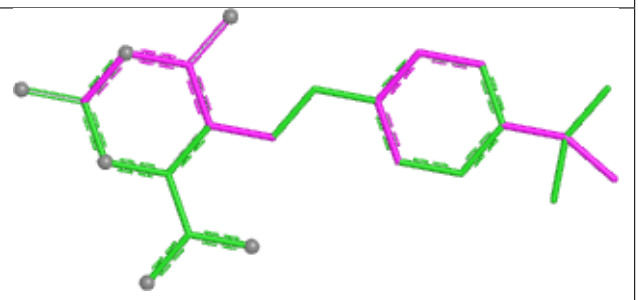
Ligand 2RO A 401



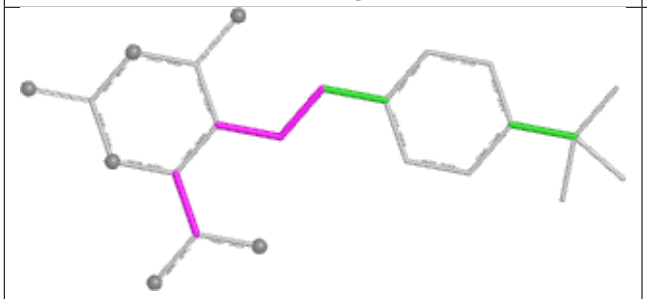
Ligand 2RO B 401



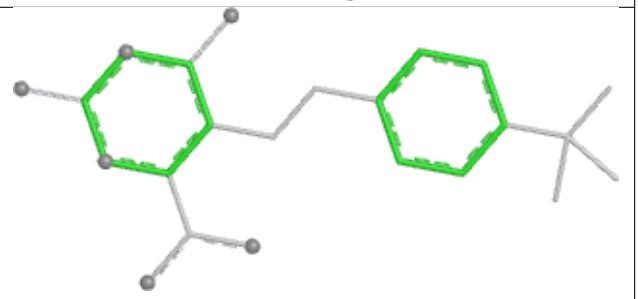
Bond lengths



Bond angles

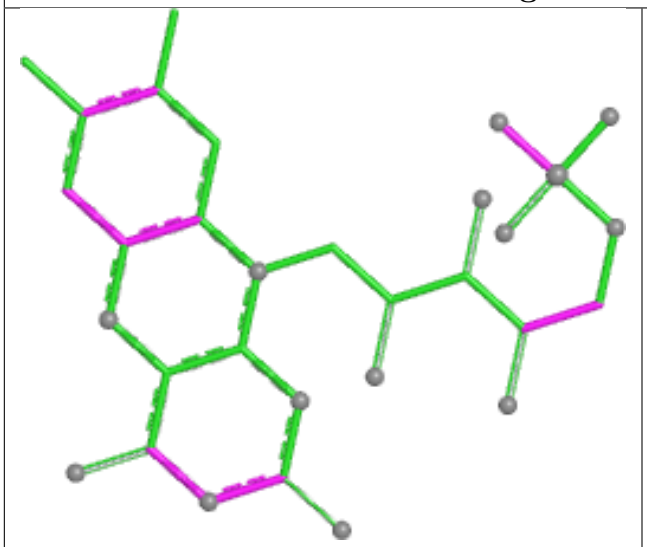


Torsions

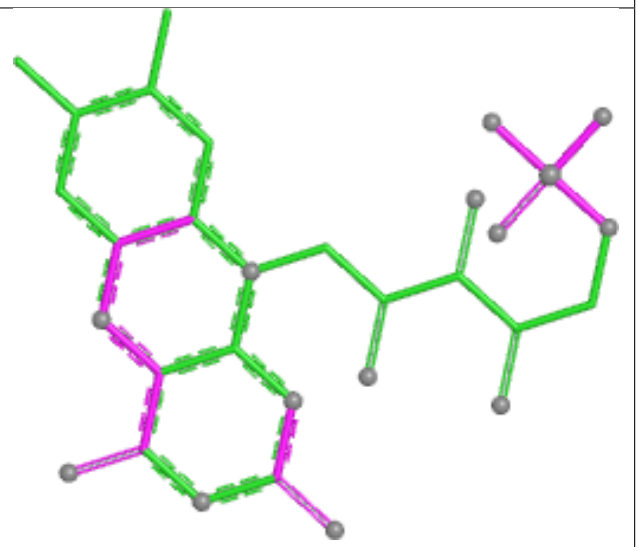


Rings

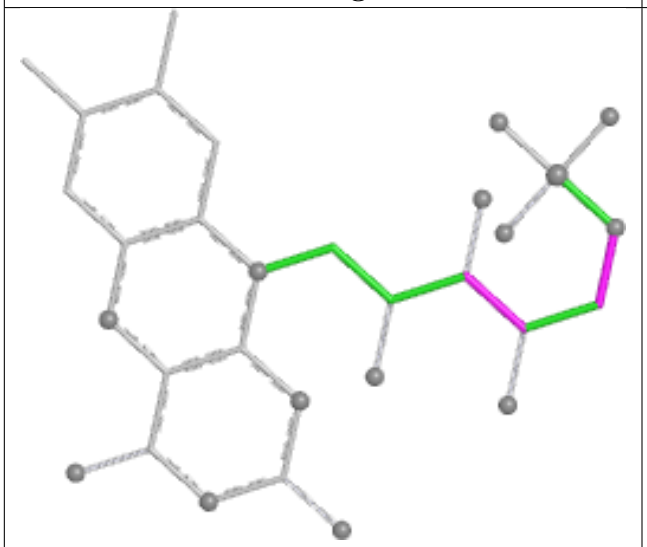
Ligand FMN A 407



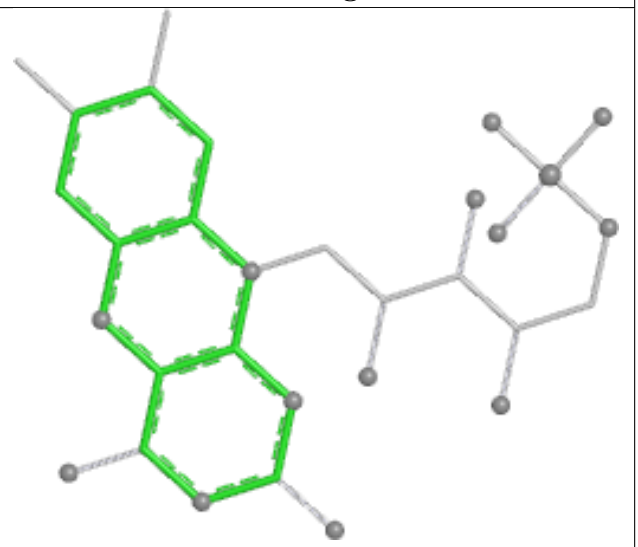
Bond lengths



Bond angles

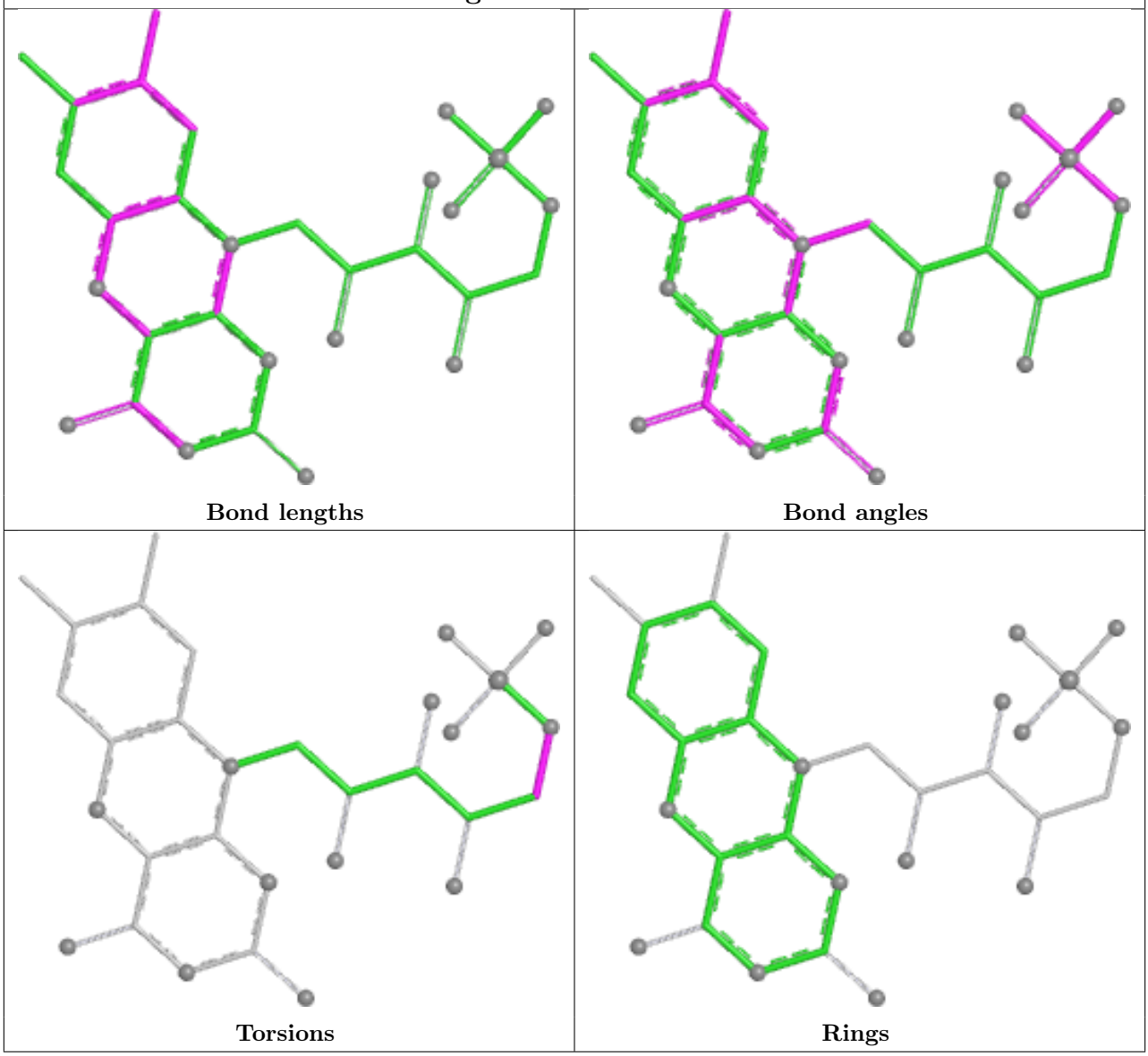


Torsions



Rings

Ligand FMN B 403



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	313/313 (100%)	0.04	7 (2%)	62	71	13, 20, 38, 58	0
1	B	313/313 (100%)	0.17	11 (3%)	47	57	13, 21, 43, 75	0
All	All	626/626 (100%)	0.11	18 (2%)	53	63	13, 21, 39, 75	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	133	VAL	6.0
1	B	134	PRO	5.0
1	B	135	GLY	4.8
1	B	0	MET	4.3
1	A	144	GLU	3.5
1	B	137	PRO	3.3
1	A	133	VAL	3.0
1	B	6	LEU	3.0
1	A	130	CYS	3.0
1	A	131	PRO	3.0
1	B	149	TYR	2.9
1	B	1	CYS	2.7
1	A	132	ASN	2.7
1	A	302	GLU	2.2
1	B	312	GLU	2.2
1	A	119	GLU	2.2
1	B	131	PRO	2.2
1	B	155	LEU	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 oligosaccharides in this entry.

6.4 Ligands (i)

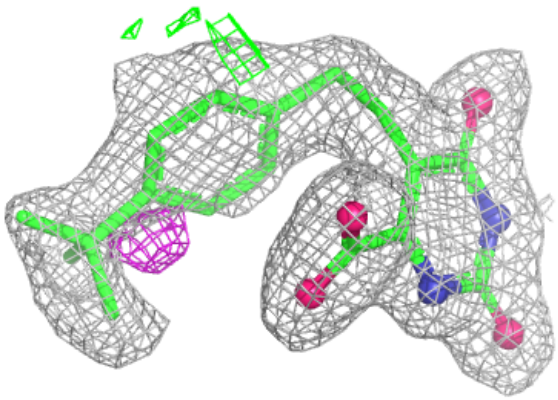
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

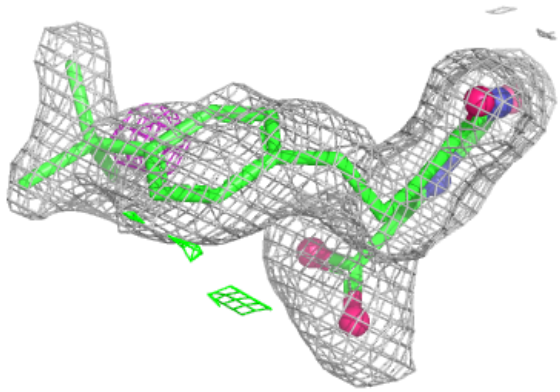
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	GOL	A	405	6/6	0.84	0.19	30,38,43,46	0
3	GOL	A	402	6/6	0.86	0.11	23,30,32,34	0
3	GOL	B	402	6/6	0.88	0.14	33,36,38,38	0
3	GOL	A	404	6/6	0.91	0.07	28,30,32,34	0
2	2RO	A	401	23/23	0.92	0.10	16,19,37,40	0
3	GOL	A	406	6/6	0.93	0.08	33,35,36,38	0
2	2RO	B	401	23/23	0.93	0.11	17,19,45,47	0
3	GOL	A	403	6/6	0.94	0.07	26,26,28,28	0
4	FMN	A	407	31/31	0.97	0.05	11,14,17,18	0
4	FMN	B	403	31/31	0.97	0.05	11,15,17,19	0
5	NCO	A	408	7/7	0.99	0.07	16,17,17,17	0

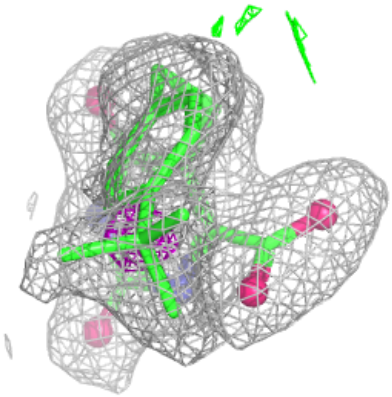
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 2RO A 401:

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

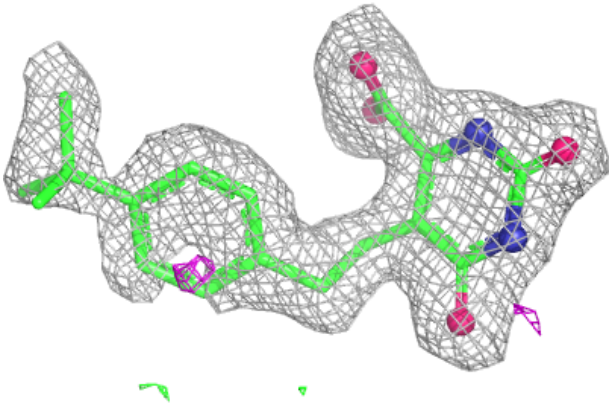


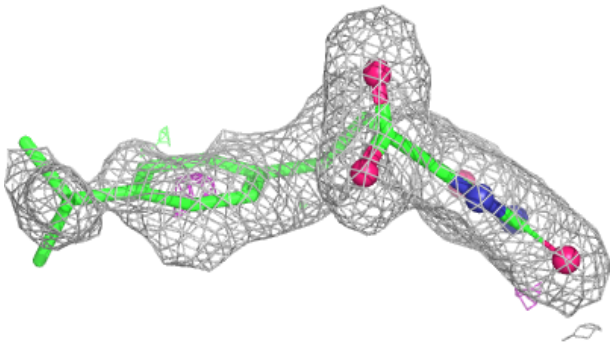


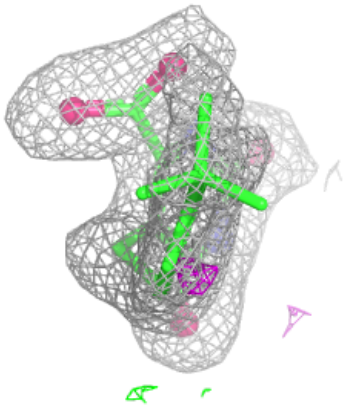


Electron density around 2RO B 401:

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

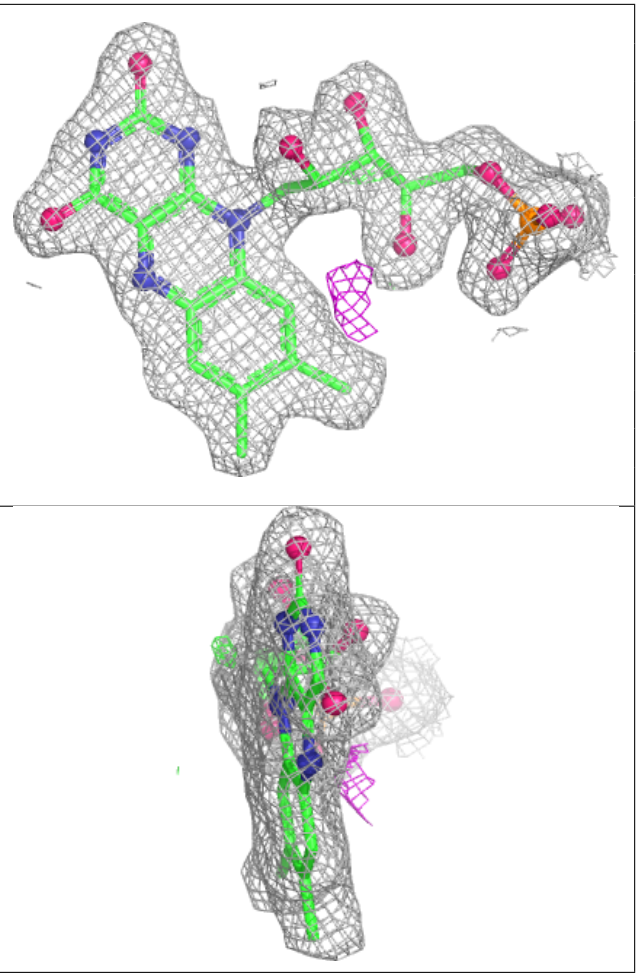






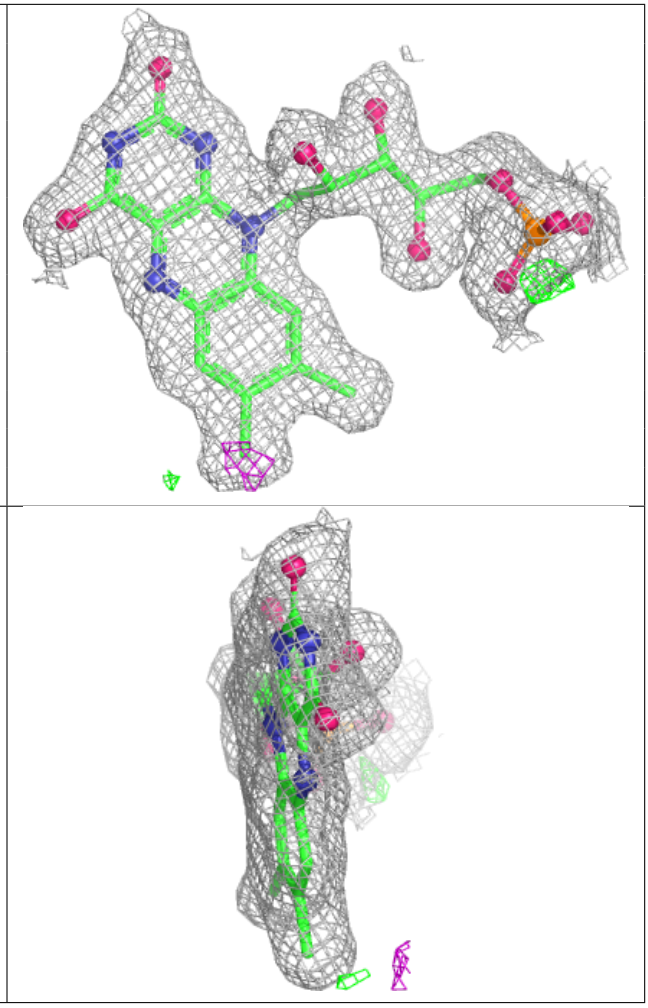
Electron density around FMN A 407:

$2mF_o$-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 403:

$2mF_o$-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.