Full wwPDB X-ray Structure Validation Report (i)

Aug 4, 2026 – 06:00 PM EDT

PDB ID	:	3W85 / pdb_00003w85
Title	:	Structure of Trypanosoma cruzi dihydroorotate dehydrogenase in complex with TT2-3-139
Authors	:	Inaoka, D.K.; Iida, M.; Tabuchi, T.; Lee, N.; Hashimoto, S.; Matsuoka, S.; Kuranaga, T.; 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	:	2013-03-12
Resolution	:	2.00 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 (1)) were used in the production of this report:

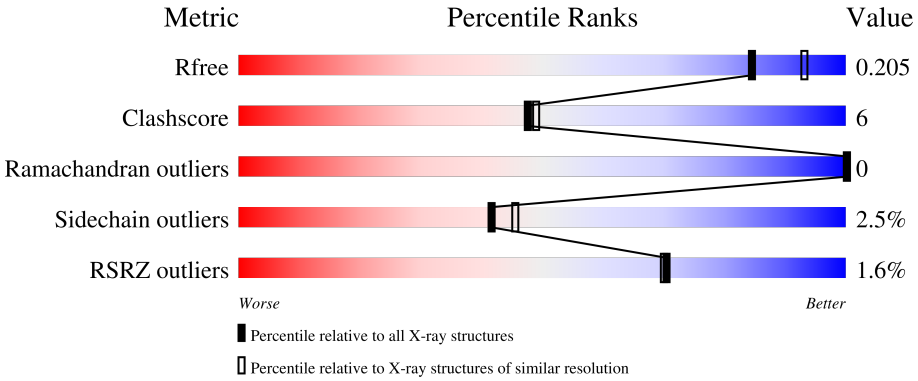
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 2.00 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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% 83% 14%
1	B	313	2% 87% 12%

2 Entry composition

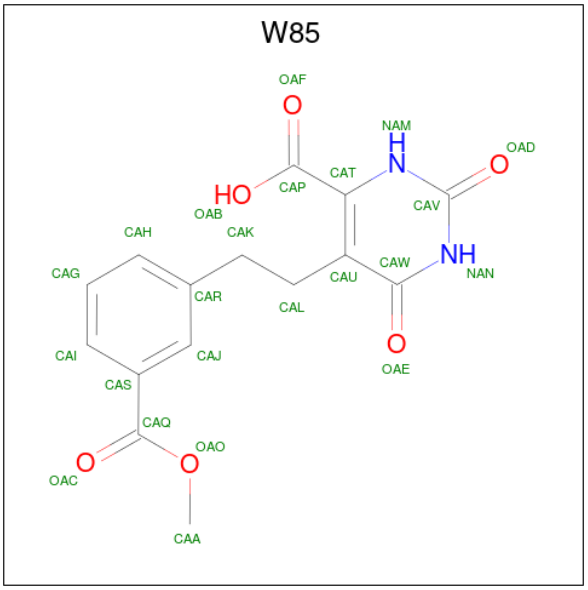
There are 6 unique types of molecules in this entry. The entry contains 5461 atoms, of which 0 are hydrogens and 0 are deuteriums.

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).

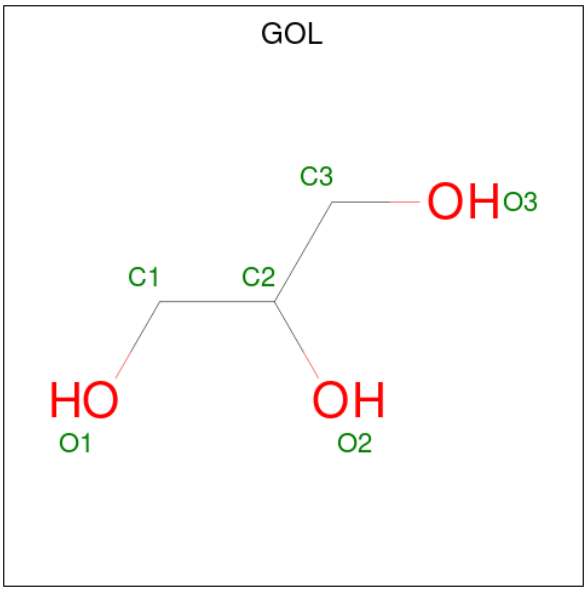
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	313	Total	C	N	O	S	0	3	0
			2416	1545	405	448	18			
1	B	313	Total	C	N	O	S	0	6	0
			2439	1562	407	452	18			

- Molecule 2 is 5-{2-[3-(methoxycarbonyl)phenyl]ethyl}-2,6-dioxo-1,2,3,6-tetrahydropyrimidine-4-carboxylic acid (CCD ID: W85) (formula: $C_{15}H_{14}N_2O_6$).



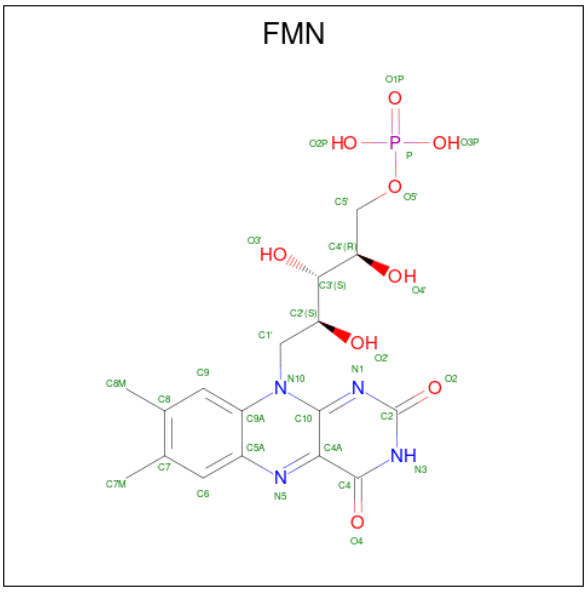
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			23	15	2	6		
2	B	1	Total	C	N	O	0	0
			23	15	2	6		

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



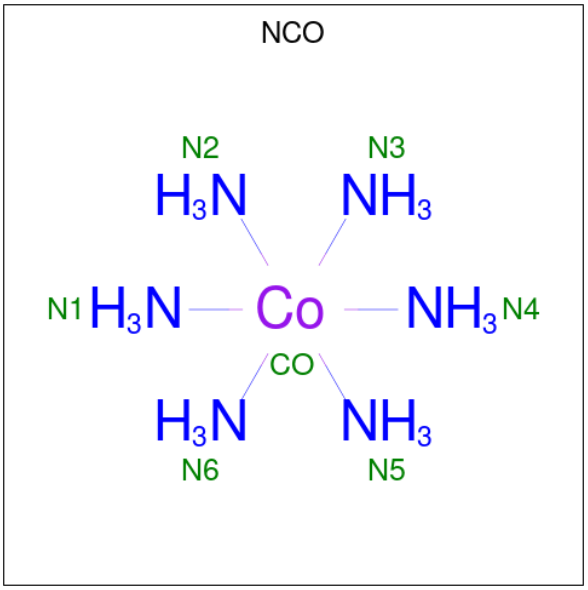
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 6 3 3	0	0
3	A	1	Total C O 6 3 3	0	0
3	A	1	Total C O 6 3 3	0	0
3	A	1	Total C O 6 3 3	0	0
3	A	1	Total C O 6 3 3	0	0
3	A	1	Total C O 6 3 3	0	0
3	A	1	Total C O 6 3 3	0	0
3	A	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0

- 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			

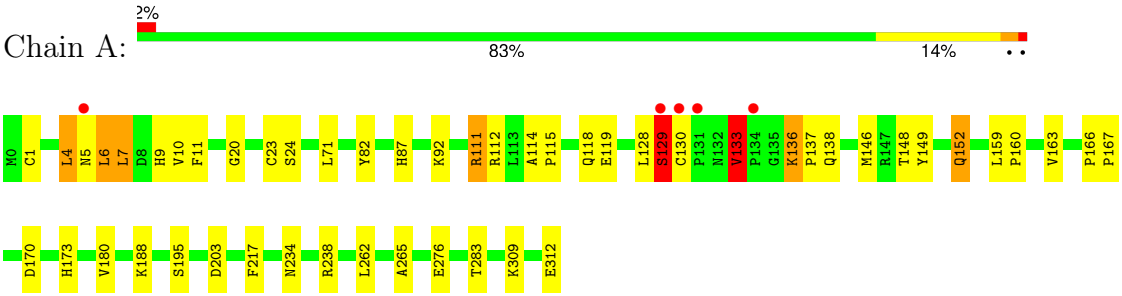
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	224	Total O 227 227	0	3
6	B	207	Total O 210 210	0	3

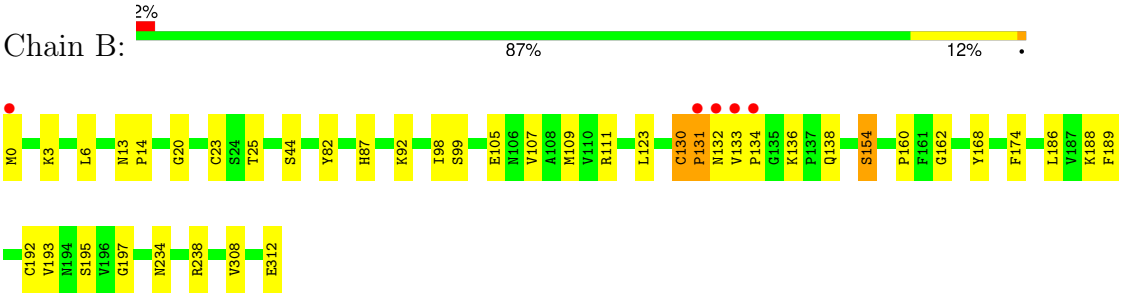
3 Residue-property plots (i)

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)



• Molecule 1: Dihydroorotate dehydrogenase (fumarate)



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	68.26Å 72.06Å 129.44Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.97 – 2.00 46.97 – 2.00	Depositor EDS
% Data completeness (in resolution range)	98.6 (46.97-2.00) 98.6 (46.97-2.00)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.28 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.154 , 0.202 0.157 , 0.205	Depositor DCC
R_{free} test set	2167 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å^2)	17.5	Xtriage
Anisotropy	0.087	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 38.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	5461	wwPDB-VP
Average B, all atoms (Å^2)	20.0	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 31.44 % 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 1.1059e-03. 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: W85, NCO, GOL, FMN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	1.42	17/2468 (0.7%)	1.24	15/3341 (0.4%)
1	B	1.30	8/2491 (0.3%)	1.17	4/3373 (0.1%)
All	All	1.36	25/4959 (0.5%)	1.20	19/6714 (0.3%)

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	111[A]	ARG	C-O	-9.11	1.13	1.24
1	A	111[B]	ARG	C-O	-9.11	1.13	1.24
1	A	23	CYS	C-O	-7.26	1.16	1.24
1	B	23	CYS	C-O	-6.48	1.17	1.24
1	A	130	CYS	C-N	6.46	1.42	1.33
1	A	265	ALA	C-O	-6.37	1.16	1.23
1	A	129	SER	CA-C	-5.91	1.46	1.53
1	A	112	ARG	C-O	-5.91	1.17	1.24
1	B	130	CYS	C-N	5.74	1.41	1.33
1	A	133	VAL	C-N	5.66	1.41	1.33
1	A	4	LEU	C-O	-5.64	1.17	1.23
1	B	123	LEU	C-O	-5.56	1.17	1.23
1	A	136	LYS	C-N	5.54	1.40	1.33
1	A	137	PRO	N-CD	5.45	1.55	1.47
1	B	308	VAL	C-O	5.45	1.29	1.24
1	B	133	VAL	C-N	5.37	1.40	1.33
1	A	167	PRO	C-O	5.29	1.29	1.23
1	A	7	LEU	C-O	-5.24	1.16	1.23
1	A	283	THR	N-CA	5.21	1.52	1.46
1	A	1	CYS	C-O	-5.19	1.17	1.23
1	B	131	PRO	N-CD	5.18	1.55	1.47
1	A	24	SER	C-O	-5.09	1.17	1.24
1	B	134	PRO	N-CD	5.09	1.54	1.47
1	A	276	GLU	C-O	-5.07	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	25	THR	C-O	-5.04	1.17	1.23

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	111[A]	ARG	CA-C-N	8.90	132.93	120.29
1	A	111[A]	ARG	C-N-CA	8.90	132.93	120.29
1	A	111[B]	ARG	CA-C-N	8.90	132.93	120.29
1	A	111[B]	ARG	C-N-CA	8.90	132.93	120.29
1	A	24	SER	N-CA-C	7.16	120.50	111.69
1	A	136	LYS	CA-C-N	-6.80	113.29	120.03
1	A	136	LYS	C-N-CA	-6.80	113.29	120.03
1	A	133	VAL	CA-C-N	-6.54	113.02	119.76
1	A	133	VAL	C-N-CA	-6.54	113.02	119.76
1	B	130	CYS	CA-C-N	-6.42	113.17	119.78
1	B	130	CYS	C-N-CA	-6.42	113.17	119.78
1	A	119	GLU	N-CA-C	6.30	117.94	111.14
1	B	133	VAL	CA-C-N	-6.21	113.36	119.76
1	B	133	VAL	C-N-CA	-6.21	113.36	119.76
1	A	1	CYS	N-CA-C	5.67	117.69	109.07
1	A	130	CYS	CA-C-N	-5.16	114.45	119.76
1	A	130	CYS	C-N-CA	-5.16	114.45	119.76
1	A	149	TYR	N-CA-C	-5.13	105.68	111.28
1	A	4	LEU	CA-CB-CG	5.11	134.18	116.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2416	0	2419	36	0
1	B	2439	0	2447	20	0
2	A	23	0	13	1	0
2	B	23	0	13	0	0
3	A	48	0	63	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	6	0	8	2	0
4	A	31	0	19	1	0
4	B	31	0	19	1	0
5	A	7	0	0	0	0
6	A	227	0	0	3	0
6	B	210	0	0	1	0
All	All	5461	0	5001	56	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 (56) 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:128:LEU:HD12	1:A:163:VAL:CG1	2.10	0.81
1:B:132:ASN:HB2	6:B:575:HOH:O	1.82	0.79
1:A:195:SER:O	3:A:405:GOL:H31	1.85	0.76
1:A:128:LEU:HD12	1:A:163:VAL:HG11	1.67	0.75
1:A:133:VAL:HG22	1:A:136:LYS:HG3	1.69	0.75
1:B:234:ASN:HD21	1:B:238:ARG:HE	1.32	0.74
1:A:234:ASN:HD21	1:A:238:ARG:HE	1.36	0.73
1:A:146:MET:HE2	1:A:180:VAL:CG1	2.19	0.72
1:B:130:CYS:H	1:B:138:GLN:HE22	1.37	0.72
1:B:44:SER:HB3	1:B:99:SER:HB2	1.73	0.70
1:A:5:ASN:ND2	1:A:10:VAL:HG22	2.08	0.69
1:A:118:GLN:HG2	1:A:159:LEU:HD11	1.77	0.67
1:A:128:LEU:CD1	1:A:163:VAL:CG1	2.74	0.66
1:A:129:SER:HA	1:A:138:GLN:NE2	2.10	0.66
1:A:146:MET:HE2	1:A:180:VAL:HG11	1.78	0.65
1:A:128:LEU:CD1	1:A:163:VAL:HG11	2.29	0.61
1:B:234:ASN:ND2	1:B:238:ARG:HE	2.01	0.59
1:B:20:GLY:HA3	4:B:403:FMN:N5	2.19	0.58
1:A:234:ASN:ND2	1:A:238:ARG:HE	2.03	0.57
1:A:148:THR:O	1:A:152:GLN:HG3	2.06	0.55
1:A:114:ALA:O	1:A:118:GLN:HG3	2.06	0.55
1:A:170:ASP:HB3	1:A:173:HIS:CD2	2.42	0.55
1:A:6:LEU:CD1	1:A:11:PHE:CE1	2.90	0.55
1:B:197:GLY:HA2	3:B:402:GOL:H32	1.91	0.52
1:A:87:HIS:HE1	1:A:92:LYS:O	1.93	0.52
1:A:118:GLN:CG	1:A:159:LEU:HD11	2.39	0.52
1:B:160:PRO:HB3	1:B:188:LYS:HG3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:217:PHE:CE1	3:A:404:GOL:H12	2.45	0.52
1:A:128:LEU:CD1	1:A:163:VAL:HG13	2.39	0.51
1:B:87:HIS:HE1	1:B:92:LYS:O	1.92	0.51
1:B:13:ASN:HB2	1:B:14:PRO:HD2	1.92	0.51
1:B:82:TYR:OH	1:B:87:HIS:HD2	1.94	0.49
1:A:82:TYR:OH	1:A:87:HIS:HD2	1.96	0.49
1:A:7:LEU:O	1:A:9:HIS:HD2	1.96	0.49
1:A:195:SER:HB3	6:A:718:HOH:O	2.12	0.49
1:A:6:LEU:HD12	1:A:11:PHE:CE1	2.49	0.48
1:A:129:SER:HA	1:A:138:GLN:HE21	1.76	0.48
1:A:309:LYS:NZ	6:A:697:HOH:O	2.44	0.48
1:A:71:LEU:HD22	2:A:401:W85:H8	1.97	0.47
1:A:20:GLY:HA3	4:A:410:FMN:N5	2.30	0.46
1:B:195:SER:O	3:B:402:GOL:H12	2.17	0.45
1:B:105:GLU:HG2	1:B:109:MET:HE2	1.99	0.45
1:B:130:CYS:HB2	1:B:131:PRO:CD	2.47	0.44
1:A:111[B]:ARG:NH1	6:A:691:HOH:O	2.24	0.43
1:A:152:GLN:HE21	1:A:152:GLN:HB3	1.63	0.43
1:A:160:PRO:HB3	1:A:188:LYS:HG3	1.99	0.43
1:B:98:ILE:O	1:B:98:ILE:HG13	2.17	0.43
1:A:203:ASP:HA	3:A:406:GOL:H31	2.01	0.42
1:A:129:SER:CA	1:A:138:GLN:NE2	2.82	0.42
1:A:129:SER:HB3	1:A:166:PRO:HB3	2.02	0.42
1:B:154:SER:HB3	1:B:186:LEU:HD12	2.02	0.42
1:A:114:ALA:N	1:A:115:PRO:HD2	2.35	0.41
1:B:192:CYS:HA	1:B:193:VAL:HA	1.93	0.41
1:B:168:TYR:HB2	1:B:174:PHE:CE1	2.56	0.41
1:B:107:VAL:O	1:B:111:ARG:HG3	2.21	0.40
1:B:162:GLY:HA3	1:B:189:PHE:CZ	2.55	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	314/313 (100%)	304 (97%)	10 (3%)	0	100	100
1	B	317/313 (101%)	308 (97%)	9 (3%)	0	100	100
All	All	631/626 (101%)	612 (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	261/258 (101%)	254 (97%)	7 (3%)	39	42
1	B	264/258 (102%)	257 (97%)	7 (3%)	39	42
All	All	525/516 (102%)	511 (97%)	14 (3%)	42	42

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LEU
1	A	6	LEU
1	A	129	SER
1	A	133	VAL
1	A	152	GLN
1	A	262	LEU
1	A	312	GLU
1	B	0	MET
1	B	3	LYS
1	B	6[A]	LEU
1	B	6[B]	LEU
1	B	136	LYS
1	B	154	SER
1	B	312	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	HIS
1	A	87	HIS
1	A	138	GLN
1	A	151	GLN
1	A	152	GLN
1	A	215	GLN
1	A	234	ASN
1	A	275	GLN
1	B	9	HIS
1	B	87	HIS
1	B	132	ASN
1	B	138	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)

14 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	$\#\|Z\|>2$
5	NCO	A	411	-	6,6,6	2.07	4 (66%)	-		
2	W85	B	401	-	24,24,24	1.77	7 (29%)	31,33,33	2.16	5 (16%)
4	FMN	B	403	-	33,33,33	1.65	6 (18%)	48,50,50	1.49	5 (10%)
3	GOL	A	407	-	5,5,5	0.43	0	5,5,5	0.60	0
3	GOL	A	409	-	5,5,5	0.51	0	5,5,5	0.39	0
3	GOL	A	403	-	5,5,5	0.17	0	5,5,5	0.97	0
3	GOL	A	405	-	5,5,5	0.74	0	5,5,5	1.05	1 (20%)
3	GOL	A	404	-	5,5,5	0.23	0	5,5,5	0.56	0
3	GOL	A	406	-	5,5,5	0.36	0	5,5,5	0.26	0
3	GOL	A	408	-	5,5,5	0.89	0	5,5,5	0.75	0
4	FMN	A	410	-	33,33,33	1.36	3 (9%)	48,50,50	1.53	10 (20%)
3	GOL	B	402	-	5,5,5	0.70	0	5,5,5	1.01	0
2	W85	A	401	-	24,24,24	2.04	7 (29%)	31,33,33	1.91	8 (25%)
3	GOL	A	402	-	5,5,5	1.15	0	5,5,5	0.94	0

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
2	W85	B	401	-	-	3/15/15/15	0/2/2/2
4	FMN	B	403	-	-	1/18/18/18	0/3/3/3
3	GOL	A	407	-	-	2/4/4/4	-
3	GOL	A	409	-	-	2/4/4/4	-
3	GOL	A	403	-	-	0/4/4/4	-
3	GOL	A	405	-	-	4/4/4/4	-
3	GOL	A	404	-	-	0/4/4/4	-
3	GOL	A	406	-	-	0/4/4/4	-
3	GOL	A	408	-	-	0/4/4/4	-
4	FMN	A	410	-	-	2/18/18/18	0/3/3/3
3	GOL	B	402	-	-	4/4/4/4	-
2	W85	A	401	-	-	4/15/15/15	0/2/2/2
3	GOL	A	402	-	-	0/4/4/4	-

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	403	FMN	C9A-C5A	5.24	1.49	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	W85	CAK-CAR	-4.39	1.39	1.51
4	A	410	FMN	C9A-C5A	4.01	1.47	1.41
2	B	401	W85	CAK-CAR	-3.93	1.40	1.51
4	B	403	FMN	C4-N3	-3.57	1.32	1.38
4	A	410	FMN	C5'-C4'	3.55	1.56	1.51
2	A	401	W85	CAW-NAN	3.43	1.45	1.38
2	A	401	W85	CAL-CAU	-3.34	1.42	1.51
4	A	410	FMN	C8-C7	3.28	1.48	1.40
4	B	403	FMN	C8-C7	3.18	1.48	1.40
2	A	401	W85	CAV-NAM	3.11	1.42	1.37
2	B	401	W85	OAF-CAP	3.07	1.30	1.22
4	B	403	FMN	C4A-N5	2.88	1.37	1.30
5	A	411	NCO	CO-N1	2.84	2.05	1.96
2	B	401	W85	CAS-CAQ	-2.81	1.43	1.50
2	A	401	W85	CAS-CAQ	-2.80	1.43	1.50
2	B	401	W85	CAJ-CAS	2.79	1.43	1.39
2	B	401	W85	CAT-NAM	2.54	1.43	1.38
4	B	403	FMN	C5'-C4'	2.50	1.55	1.51
4	B	403	FMN	O4-C4	2.50	1.28	1.23
5	A	411	NCO	CO-N6	2.35	2.04	1.96
2	B	401	W85	CAL-CAU	-2.33	1.45	1.51
2	A	401	W85	CAJ-CAS	2.32	1.43	1.39
2	A	401	W85	OAO-CAQ	2.27	1.38	1.33
5	A	411	NCO	CO-N4	2.25	2.04	1.96
5	A	411	NCO	CO-N2	2.17	2.03	1.96
2	B	401	W85	OAO-CAQ	2.15	1.38	1.33

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	401	W85	CAU-CAW-NAN	8.13	121.88	115.70
2	A	401	W85	CAU-CAW-NAN	5.34	119.76	115.70
2	B	401	W85	CAW-NAN-CAV	-5.32	119.04	126.37
4	A	410	FMN	O4-C4-C4A	-4.44	114.81	126.53
2	A	401	W85	OAB-CAP-CAT	4.34	123.61	116.73
2	A	401	W85	CAW-NAN-CAV	-3.96	120.92	126.37
4	B	403	FMN	C9A-C5A-N5	-3.86	118.36	122.45
4	B	403	FMN	O4-C4-N3	3.60	126.89	120.11
2	B	401	W85	OAE-CAW-CAU	-3.54	120.19	124.56
4	B	403	FMN	O4-C4-C4A	-3.54	117.20	126.53
2	A	401	W85	CAL-CAU-CAW	3.48	121.31	116.64
4	A	410	FMN	O2P-P-O1P	3.15	123.11	110.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	403	FMN	C5A-C9A-N10	3.00	120.68	117.97
2	B	401	W85	NAN-CAV-NAM	2.96	120.39	115.74
4	A	410	FMN	O4-C4-N3	2.91	125.59	120.11
2	A	401	W85	OAO-CAQ-CAS	2.88	116.62	112.31
2	B	401	W85	OAO-CAQ-CAS	2.88	116.62	112.31
4	B	403	FMN	O4'-C4'-C3'	2.86	115.94	109.25
2	A	401	W85	CAA-OAO-CAQ	-2.70	110.62	115.81
2	A	401	W85	OAE-CAW-CAU	-2.67	121.27	124.56
4	A	410	FMN	C5'-C4'-C3'	-2.53	107.45	112.22
4	A	410	FMN	O5'-C5'-C4'	2.49	116.00	109.36
4	A	410	FMN	C4A-C4-N3	2.47	119.54	113.25
2	A	401	W85	OAF-CAP-CAT	-2.44	115.95	120.20
4	A	410	FMN	C9A-C5A-N5	-2.40	119.90	122.45
4	A	410	FMN	C4-N3-C2	-2.19	121.76	125.64
4	A	410	FMN	O2'-C2'-C3'	-2.11	104.30	109.25
4	A	410	FMN	C4-C4A-N5	2.09	121.10	118.21
3	A	405	GOL	O2-C2-C3	2.04	117.61	109.18

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	W85	OAB-CAP-CAT-NAM
2	B	401	W85	OAB-CAP-CAT-NAM
3	A	405	GOL	C1-C2-C3-O3
3	A	407	GOL	O1-C1-C2-C3
3	A	409	GOL	C1-C2-C3-O3
3	B	402	GOL	C1-C2-C3-O3
3	A	405	GOL	O2-C2-C3-O3
3	B	402	GOL	O1-C1-C2-O2
3	B	402	GOL	O2-C2-C3-O3
3	A	405	GOL	O1-C1-C2-C3
3	B	402	GOL	O1-C1-C2-C3
3	A	405	GOL	O1-C1-C2-O2
3	A	407	GOL	O1-C1-C2-O2
3	A	409	GOL	O2-C2-C3-O3
4	A	410	FMN	C4'-C5'-O5'-P
4	B	403	FMN	C4'-C5'-O5'-P
4	A	410	FMN	O3'-C3'-C4'-C5'
2	A	401	W85	CAR-CAK-CAL-CAU
2	B	401	W85	OAF-CAP-CAT-CAU
2	A	401	W85	OAF-CAP-CAT-NAM

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Mol	Chain	Res	Type	Atoms
2	B	401	W85	OAF-CAP-CAT-NAM
2	A	401	W85	OAO-CAQ-CAS-CAI

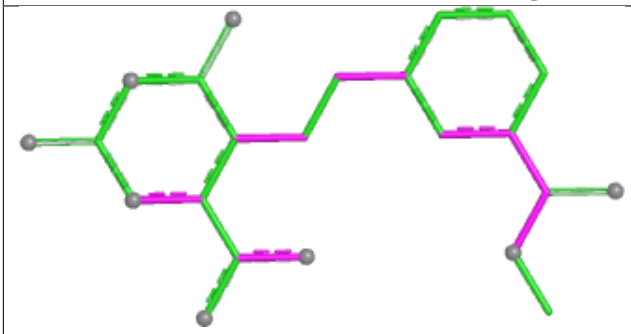
There are no ring outliers.

7 monomers are involved in 8 short contacts:

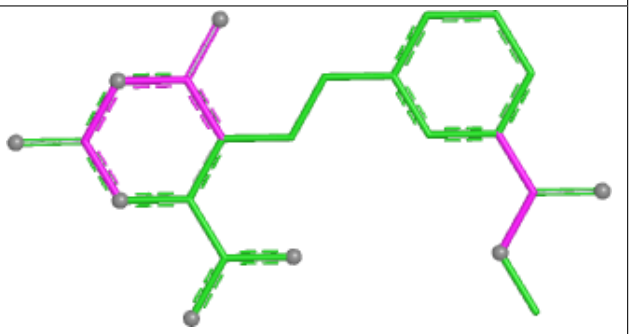
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	403	FMN	1	0
3	A	405	GOL	1	0
3	A	404	GOL	1	0
3	A	406	GOL	1	0
4	A	410	FMN	1	0
3	B	402	GOL	2	0
2	A	401	W85	1	0

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.

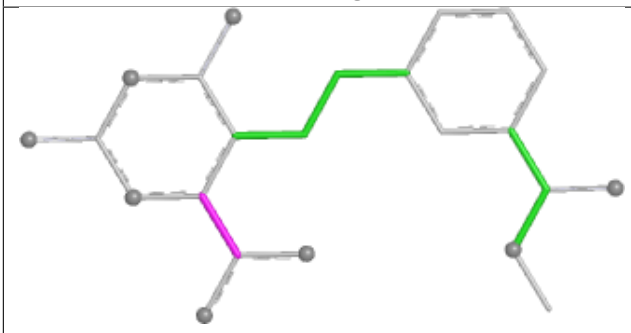
Ligand W85 B 401



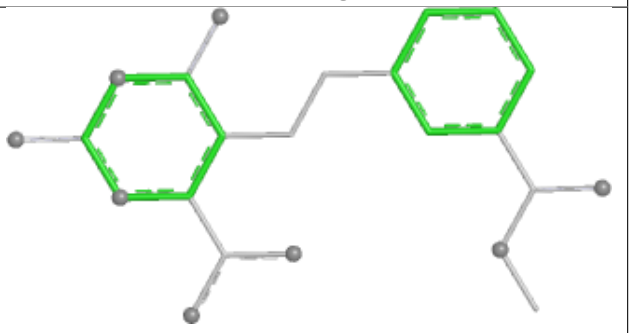
Bond lengths



Bond angles

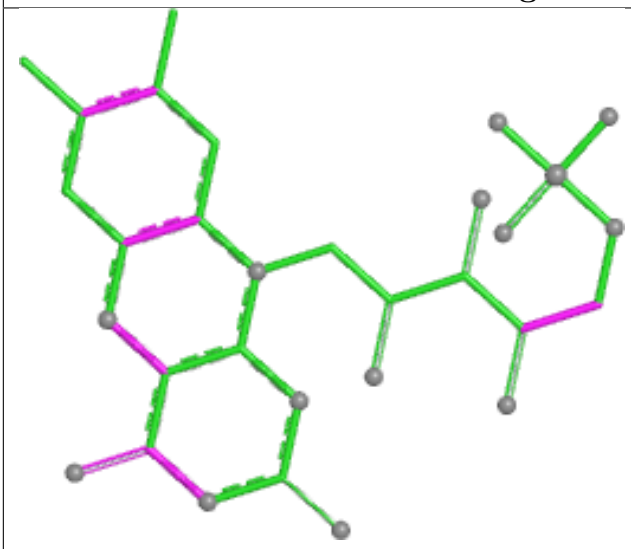


Torsions

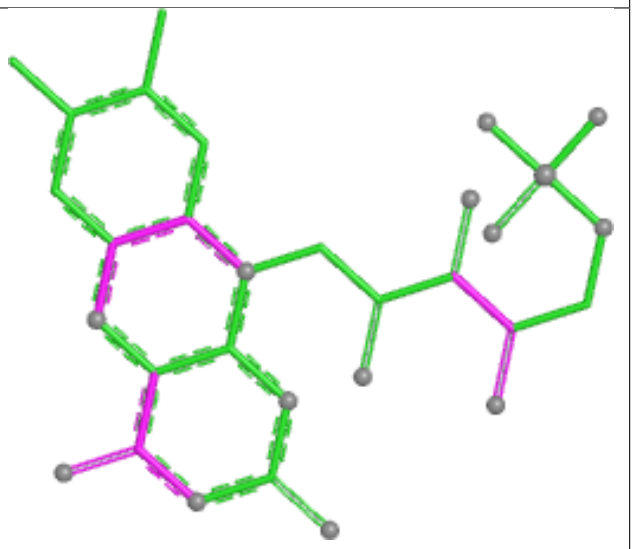


Rings

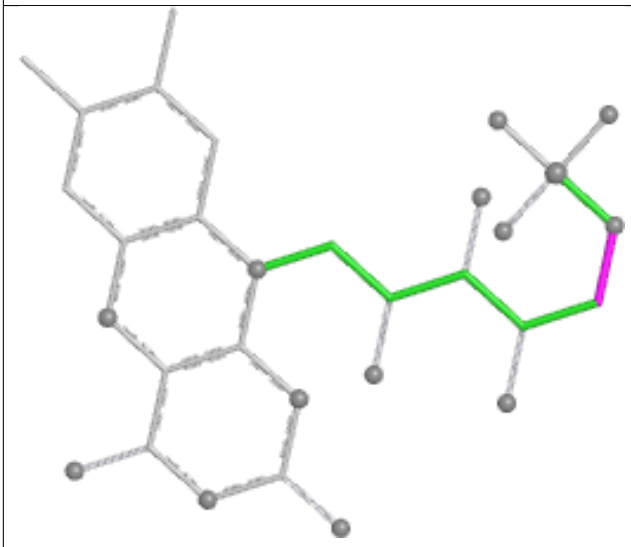
Ligand FMN B 403



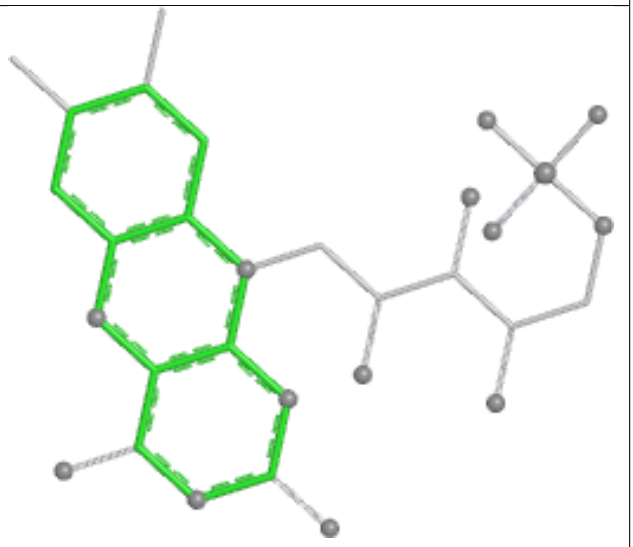
Bond lengths



Bond angles

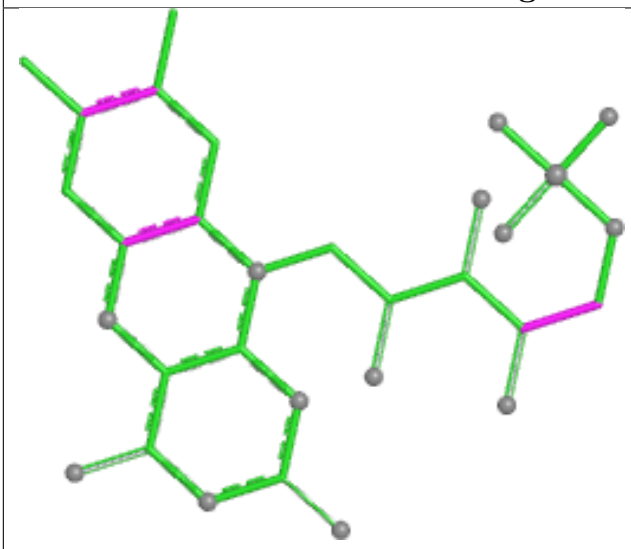


Torsions

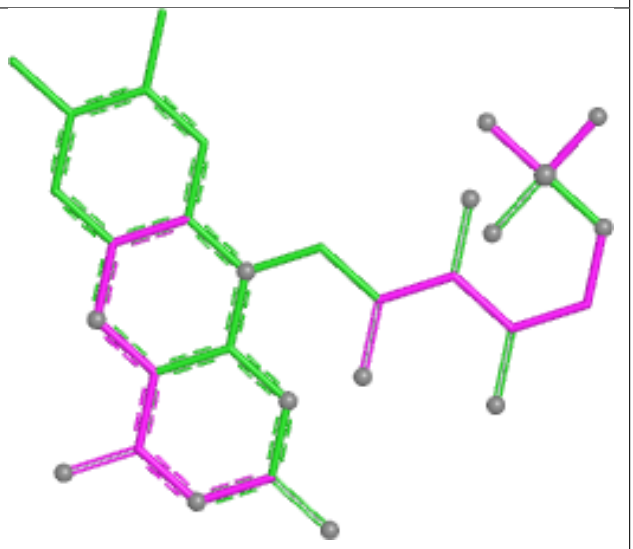


Rings

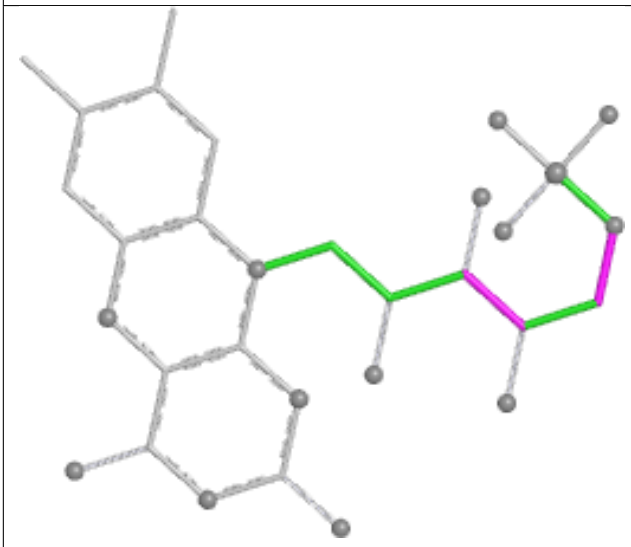
Ligand FMN A 410



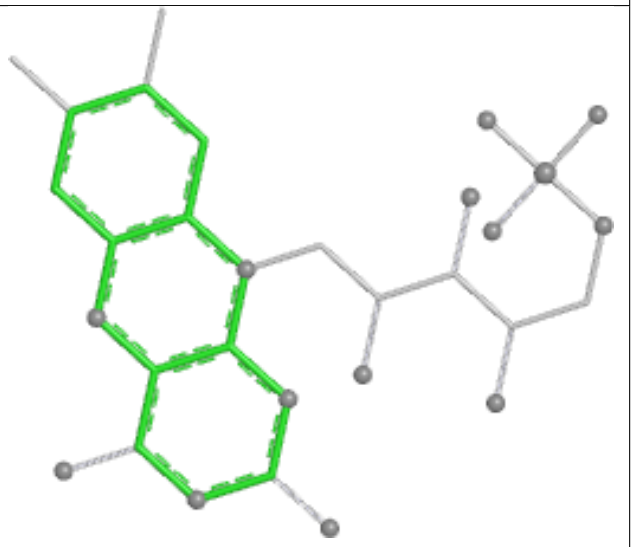
Bond lengths



Bond angles

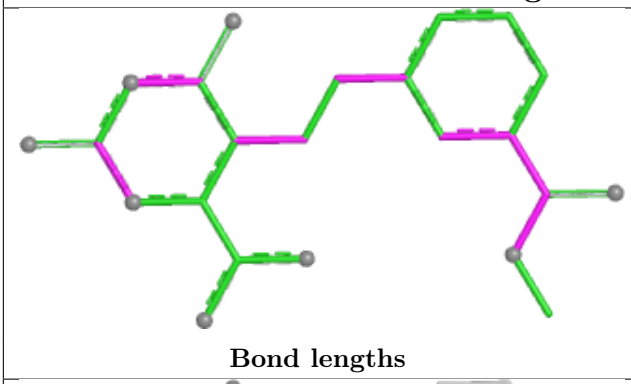


Torsions

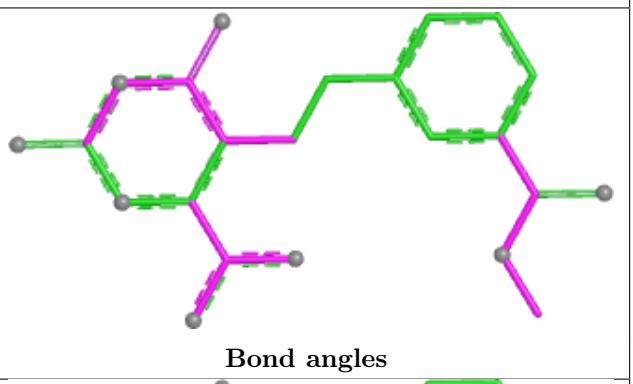


Rings

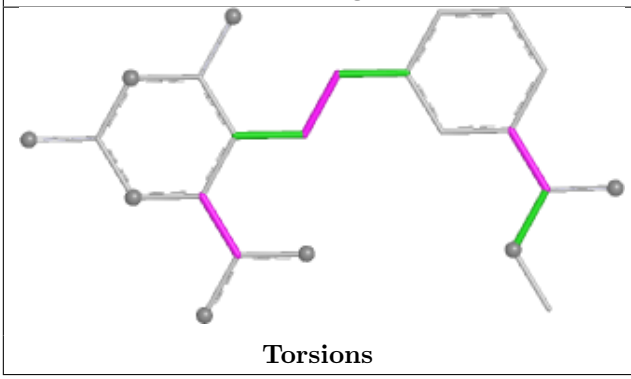
Ligand W85 A 401



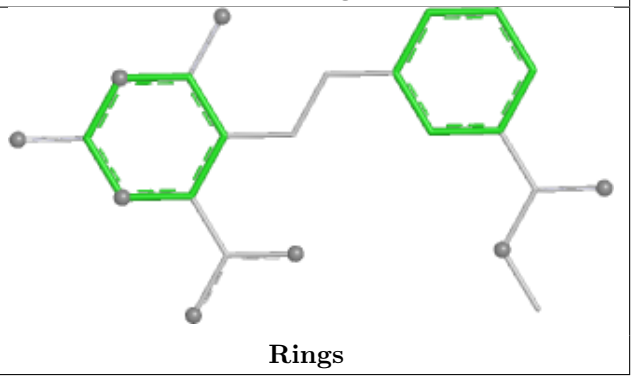
Bond lengths



Bond angles



Torsions



Rings

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

6.1 Protein, DNA and RNA chains

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%)	-0.47	5 (1%)	70	70	7, 16, 35, 54	3 (0%)
1	B	313/313 (100%)	-0.46	5 (1%)	70	70	7, 16, 35, 62	6 (1%)
All	All	626/626 (100%)	-0.47	10 (1%)	70	70	7, 16, 35, 62	9 (1%)

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	131	PRO	4.9
1	B	132	ASN	3.3
1	A	130	CYS	3.2
1	B	133	VAL	3.1
1	B	0	MET	3.0
1	A	129	SER	2.8
1	A	131	PRO	2.7
1	A	134	PRO	2.3
1	A	5	ASN	2.2
1	B	134	PRO	2.2

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no oligosaccharides in this entry.

6.4 Ligands (i)

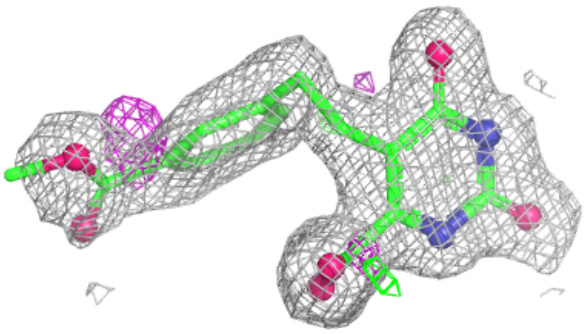
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

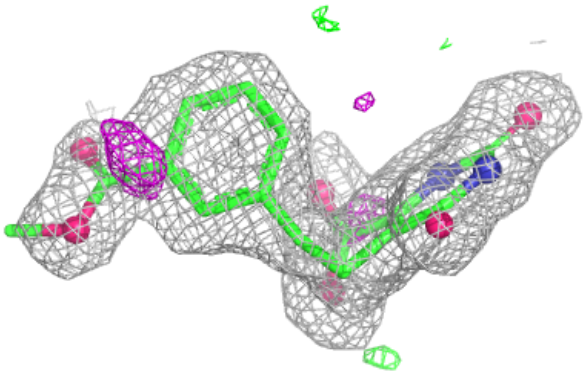
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	GOL	A	408	6/6	0.75	0.15	39,43,49,50	0
3	GOL	A	405	6/6	0.80	0.22	28,45,60,61	0
3	GOL	B	402	6/6	0.87	0.15	33,39,54,55	0
3	GOL	A	406	6/6	0.88	0.12	50,51,52,53	0
3	GOL	A	404	6/6	0.89	0.10	29,35,38,40	0
3	GOL	A	409	6/6	0.89	0.11	45,46,48,52	0
3	GOL	A	407	6/6	0.89	0.11	46,53,54,60	0
3	GOL	A	402	6/6	0.90	0.23	27,42,46,49	0
3	GOL	A	403	6/6	0.94	0.07	28,29,30,31	0
2	W85	A	401	23/23	0.94	0.08	14,20,37,44	0
2	W85	B	401	23/23	0.96	0.08	12,18,41,42	0
4	FMN	A	410	31/31	0.98	0.05	6,11,13,15	0
4	FMN	B	403	31/31	0.98	0.05	9,10,12,13	0
5	NCO	A	411	7/7	0.99	0.06	12,14,14,15	0

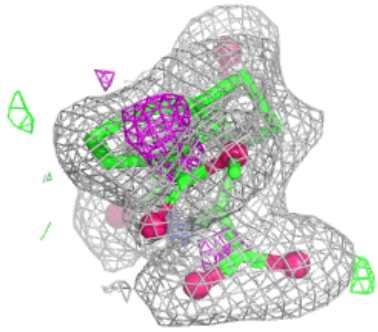
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around W85 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)

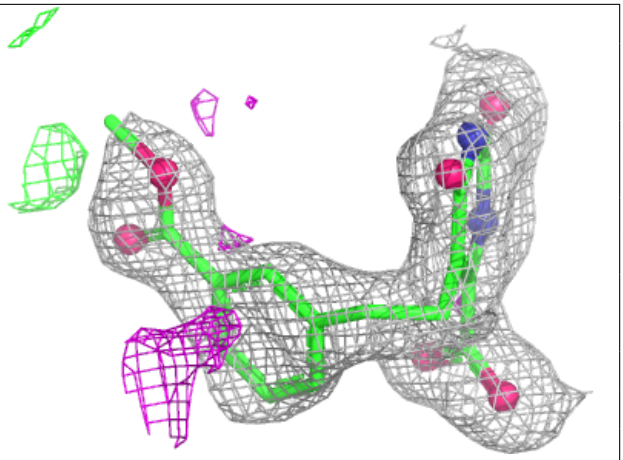


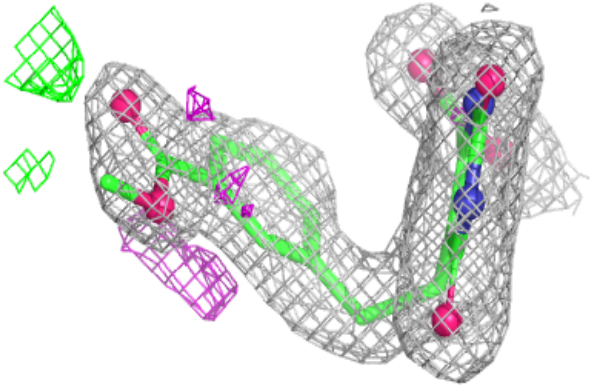


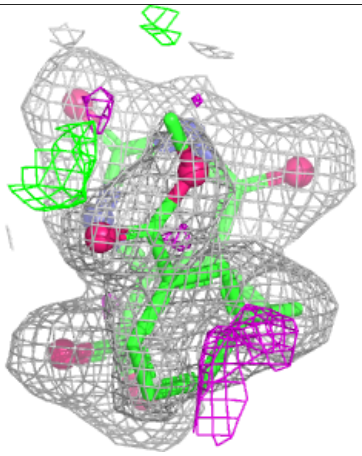


Electron density around W85 B 401:

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

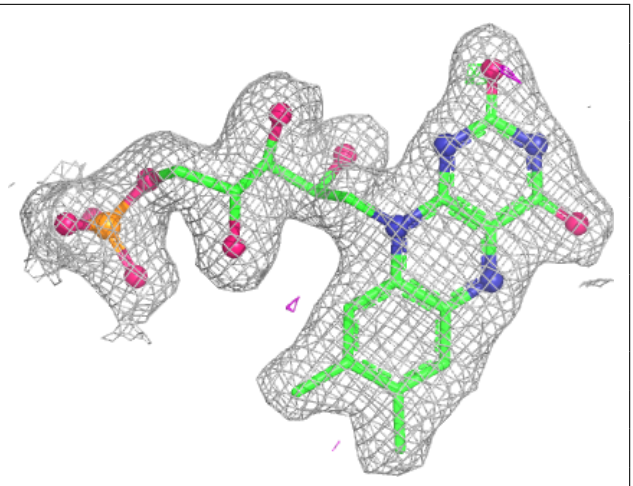


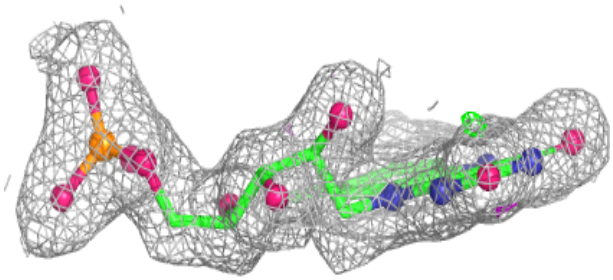




Electron density around FMN A 410:

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

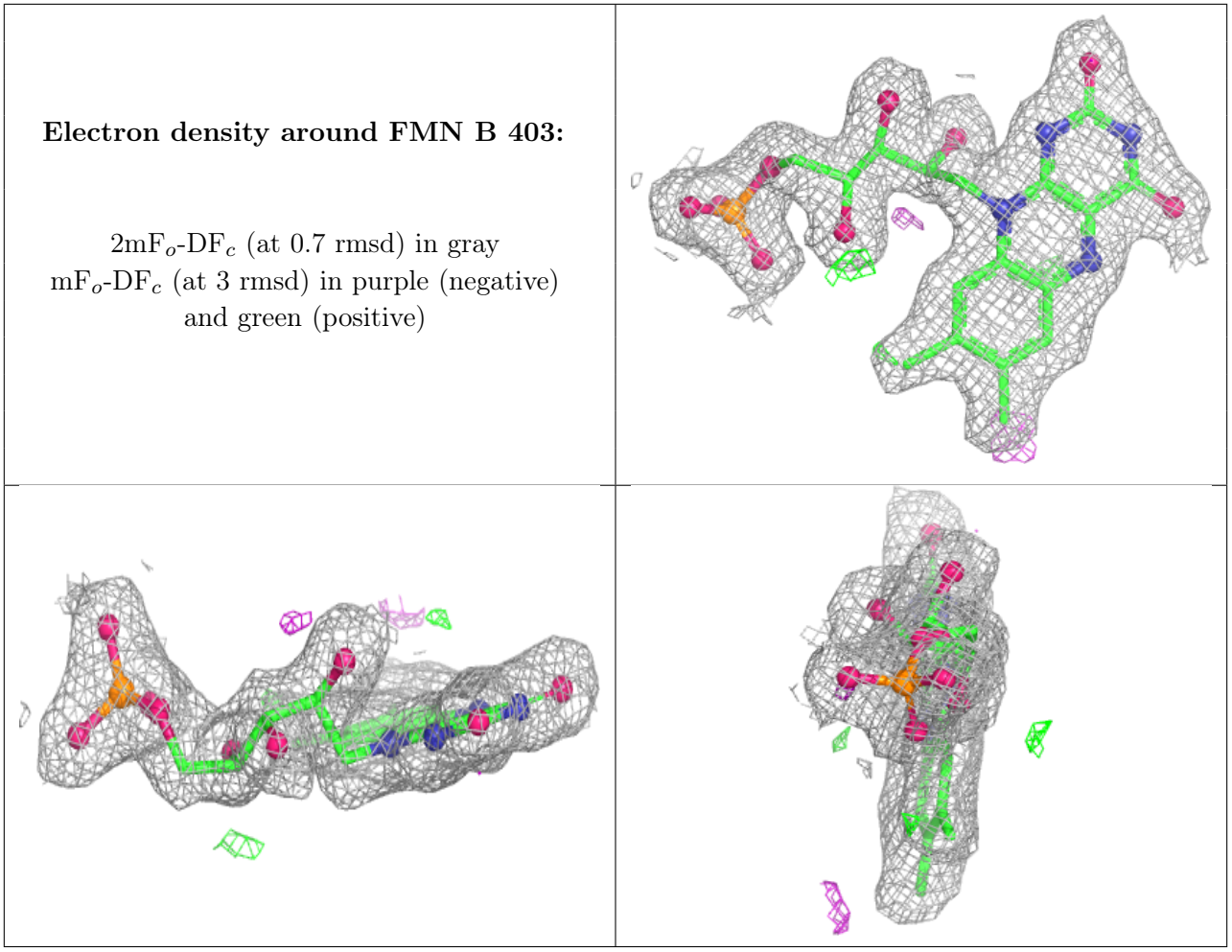






Electron density around FMN B 403:

$2mF_o$-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

There are no such residues in this entry.