Full wwPDB X-ray Structure Validation Report (i)

Aug 5, 2026 – 08:01 PM EDT

PDB ID	:	3W72 / pdb_00003w72
Title	:	Structure of Trypanosoma cruzi dihydroorotate dehydrogenase in complex with MII-4-107
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	:	2013-02-27
Resolution	:	1.55 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:

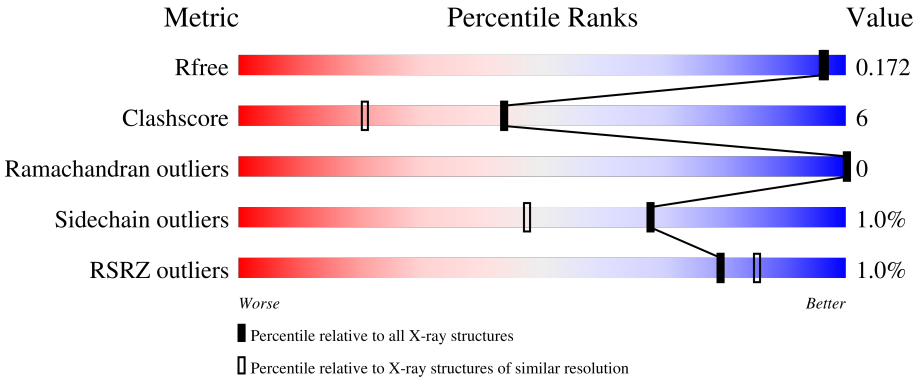
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 1.55 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	2145 (1.56-1.56)
Clashscore	190562	2189 (1.56-1.56)
Ramachandran outliers	187476	2153 (1.56-1.56)
Sidechain outliers	187428	2150 (1.56-1.56)
RSRZ outliers	180081	2146 (1.56-1.56)

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	% 84% 15% .
1	B	313	% 86% 13% ..

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	GOL	A	410	-	-	X	-
3	GOL	A	413	-	X	-	-
3	GOL	B	408	-	X	-	-

2 Entry composition

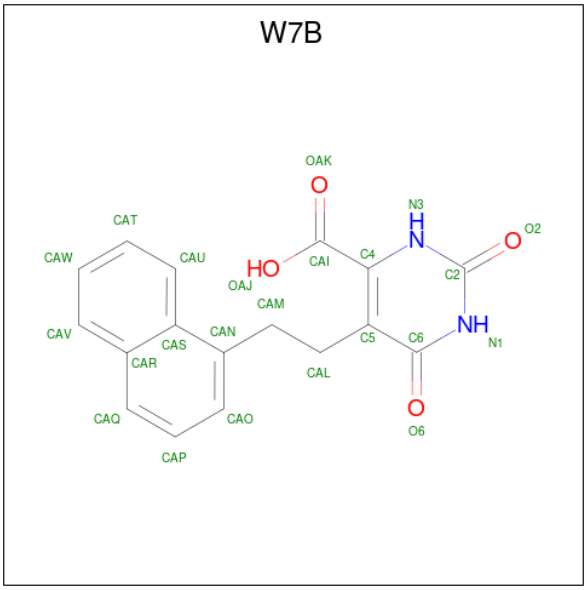
There are 6 unique types of molecules in this entry. The entry contains 5728 atoms, of which 0 are hydrogens and 0 are deuteriums.

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).

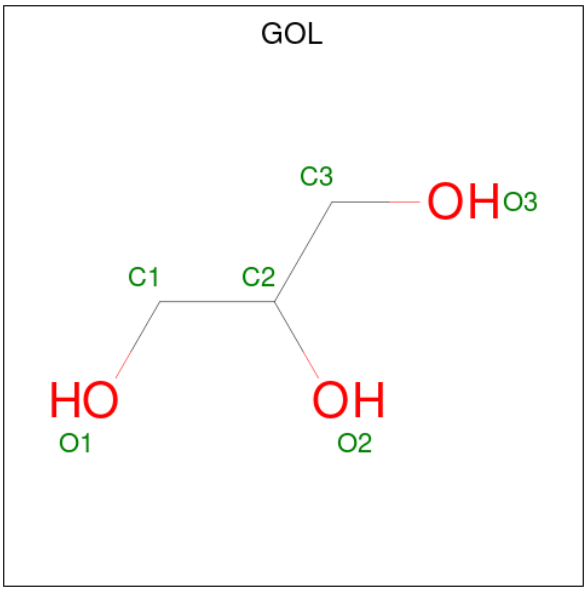
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	313	Total	C	N	O	S	0	0	0
			2388	1530	396	444	18			
1	B	313	Total	C	N	O	S	0	0	0
			2388	1530	396	444	18			

- Molecule 2 is 5-[2-(naphthalen-1-yl)ethyl]-2,6-dioxo-1,2,3,6- tetrahydropyrimidine-4-carboxy lic acid (CCD ID: W7B) (formula: $C_{17}H_{14}N_2O_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			23	17	2	4		
2	B	1	Total	C	N	O	0	1
			46	34	4	8		

- 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	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
3	B	1	Total C O 6 3 3	0	0

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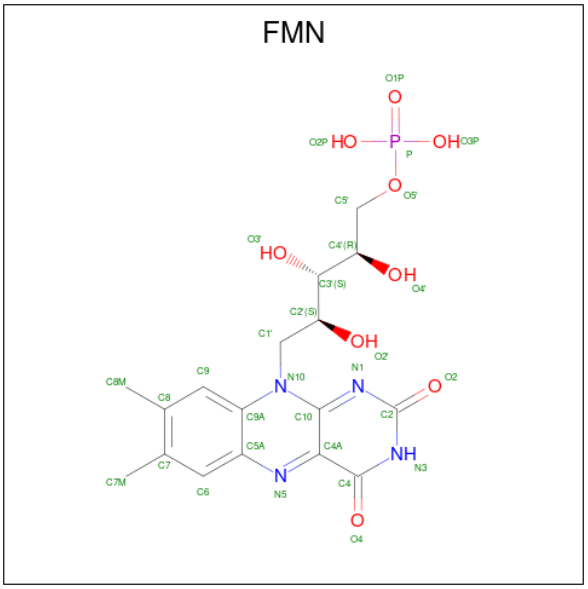
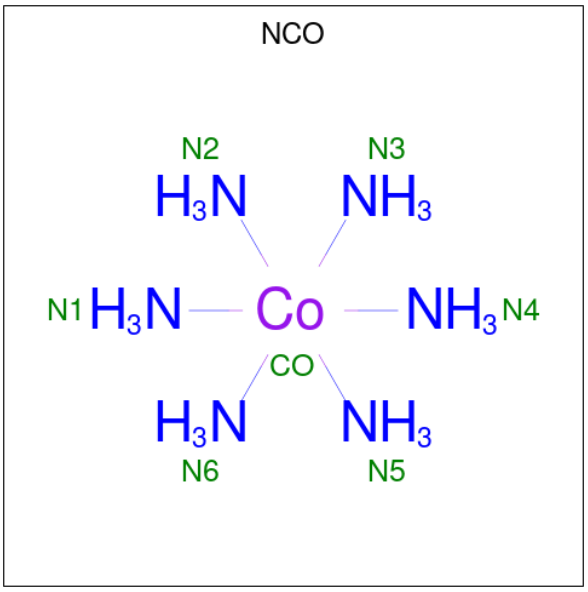
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0

- 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 31 17 4 9 1	0	0
4	B	1	Total C N O P 31 17 4 9 1	0	0

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



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

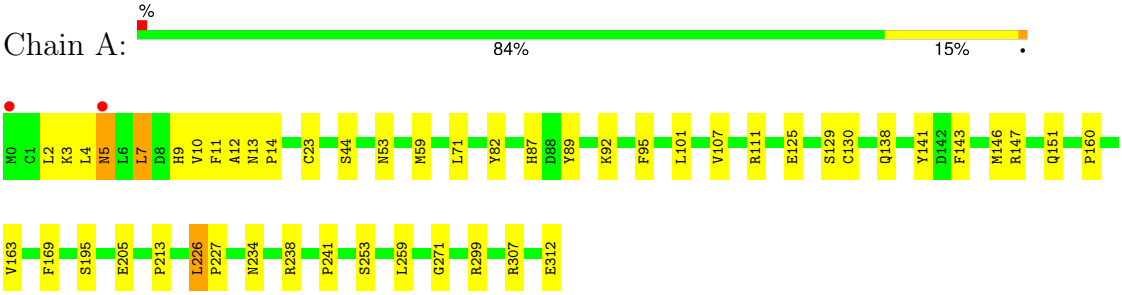
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	334	Total O 334 334	0	0
6	B	366	Total O 366 366	0	0

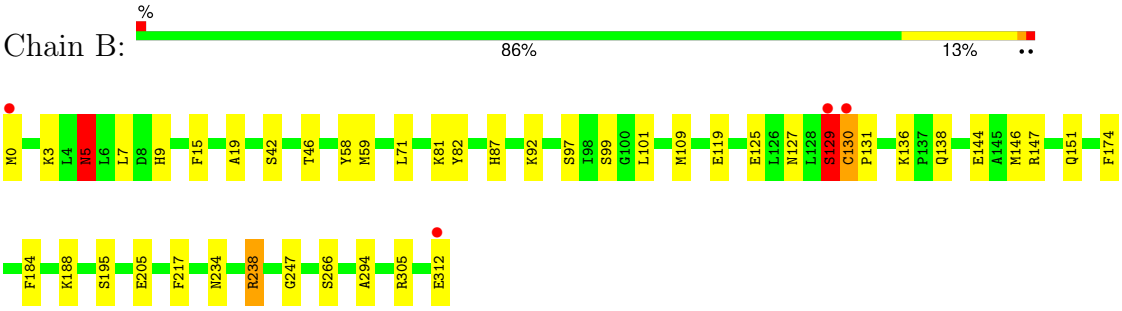
3 Residue-property plots (i)

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)



• 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	67.84Å 71.91Å 128.31Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.11 – 1.55 39.11 – 1.55	Depositor EDS
% Data completeness (in resolution range)	98.9 (39.11-1.55) 98.9 (39.11-1.55)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.40 (at 1.55Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.141 , 0.172 0.140 , 0.172	Depositor DCC
R_{free} test set	4555 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å^2)	14.1	Xtriage
Anisotropy	0.096	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 39.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	5728	wwPDB-VP
Average B, all atoms (Å^2)	16.0	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 22.70 % 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 5.4079e-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: NCO, FMN, GOL, W7B

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	1.58	18/2440 (0.7%)	1.27	5/3305 (0.2%)
1	B	1.58	19/2440 (0.8%)	1.31	8/3305 (0.2%)
All	All	1.58	37/4880 (0.8%)	1.29	13/6610 (0.2%)

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	146	MET	SD-CE	-9.41	1.56	1.79
1	A	5	ASN	CA-C	-8.98	1.42	1.52
1	A	271	GLY	CA-C	-8.10	1.46	1.51
1	B	144	GLU	C-O	-7.94	1.14	1.24
1	A	11	PHE	C-O	-7.19	1.15	1.24
1	A	253	SER	CA-C	-7.13	1.43	1.52
1	B	19	ALA	N-CA	-7.08	1.37	1.46
1	A	125	GLU	C-O	-6.92	1.16	1.24
1	B	130	CYS	CA-C	6.80	1.59	1.52
1	A	146	MET	C-O	-6.59	1.16	1.24
1	A	160	PRO	CA-CB	-6.45	1.45	1.53
1	B	205	GLU	C-O	-6.40	1.16	1.24
1	A	95	PHE	N-CA	-6.15	1.38	1.46
1	B	129	SER	CA-C	-6.10	1.47	1.53
1	B	42	SER	CA-C	-6.03	1.44	1.53
1	A	163	VAL	C-O	-5.76	1.18	1.24
1	B	15	PHE	N-CA	5.74	1.53	1.46
1	B	3	LYS	C-O	-5.71	1.16	1.23
1	B	129	SER	C-O	-5.69	1.14	1.23
1	A	226	LEU	N-CA	5.57	1.51	1.46
1	A	205	GLU	C-O	-5.54	1.17	1.24
1	B	147	ARG	C-O	-5.43	1.17	1.24
1	A	2	LEU	N-CA	5.29	1.52	1.46
1	B	5	ASN	CG-OD1	5.29	1.33	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	23	CYS	N-CA	-5.25	1.42	1.47
1	B	247	GLY	CA-C	-5.24	1.48	1.52
1	A	12	ALA	N-CA	5.24	1.53	1.46
1	B	136	LYS	C-O	-5.23	1.18	1.24
1	B	305	ARG	N-CA	-5.19	1.39	1.46
1	A	259	LEU	C-O	-5.19	1.18	1.24
1	B	238	ARG	N-CA	5.18	1.52	1.46
1	A	160	PRO	N-CA	5.15	1.53	1.47
1	B	109	MET	C-O	-5.15	1.18	1.24
1	A	146	MET	SD-CE	-5.14	1.66	1.79
1	A	7	LEU	CA-C	5.12	1.60	1.53
1	B	127	ASN	CG-OD1	-5.05	1.14	1.23
1	B	266	SER	C-O	5.05	1.30	1.24

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	129	SER	N-CA-C	-7.78	98.75	109.71
1	A	130	CYS	CA-C-N	-7.28	113.17	120.31
1	A	130	CYS	C-N-CA	-7.28	113.17	120.31
1	A	271	GLY	N-CA-C	7.22	116.78	110.21
1	B	3	LYS	CD-CE-NZ	6.24	131.88	111.90
1	A	4	LEU	CA-C-O	-5.60	115.46	121.45
1	A	307	ARG	CG-CD-NE	-5.49	99.93	112.00
1	B	5	ASN	CB-CA-C	-5.49	102.34	110.62
1	B	184	PHE	CA-C-N	5.45	125.12	119.56
1	B	184	PHE	C-N-CA	5.45	125.12	119.56
1	B	130	CYS	N-CA-CB	-5.39	100.62	110.65
1	B	131	PRO	N-CA-C	5.20	119.48	111.21
1	B	174	PHE	CA-CB-CG	5.14	118.94	113.80

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	28	0
2	A	23	0	13	0	0
2	B	46	0	26	6	0
3	A	72	0	95	12	0
3	B	42	0	56	5	0
4	A	31	0	19	0	0
4	B	31	0	19	0	0
5	B	7	0	0	0	0
6	A	334	0	0	7	0
6	B	366	0	0	11	0
All	All	5728	0	5010	61	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 (61) 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:9:HIS:CE1	3:A:410:GOL:H11	2.01	0.95
1:A:9:HIS:ND1	3:A:410:GOL:H11	1.88	0.88
3:A:412:GOL:O1	3:B:408:GOL:H2	1.77	0.85
1:B:129:SER:HA	1:B:138:GLN:OE1	1.76	0.84
1:B:59:MET:CE	6:B:844:HOH:O	2.32	0.78
3:A:410:GOL:H31	6:A:611:HOH:O	1.86	0.76
1:A:234:ASN:HD21	1:A:238:ARG:HE	1.33	0.75
1:B:5:ASN:HB3	6:B:697:HOH:O	1.88	0.74
1:B:59:MET:HE3	6:B:844:HOH:O	1.88	0.71
1:A:195:SER:HB3	6:A:725:HOH:O	1.91	0.70
1:A:9:HIS:CE1	3:A:410:GOL:C1	2.73	0.69
1:B:234:ASN:HD21	1:B:238:ARG:HE	1.42	0.68
1:A:7:LEU:O	1:A:9:HIS:HD2	1.77	0.66
1:A:59:MET:HE3	6:A:734:HOH:O	1.97	0.64
1:A:82:TYR:OH	1:A:87:HIS:HD2	1.81	0.62
1:A:241:PRO:HA	3:A:405:GOL:H12	1.82	0.62
1:B:7:LEU:O	1:B:9:HIS:HD2	1.83	0.61
1:B:82:TYR:OH	1:B:87:HIS:HD2	1.83	0.61
1:B:130:CYS:SG	2:B:401[B]:W7B:CAP	2.90	0.60
1:B:195:SER:HB3	6:B:652:HOH:O	2.04	0.58
1:A:59:MET:CE	6:A:734:HOH:O	2.51	0.58
1:B:101:LEU:HD21	2:B:401[B]:W7B:H12	1.86	0.57
1:A:143:PHE:CE2	3:A:412:GOL:H31	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:87:HIS:HE1	1:A:92:LYS:O	1.89	0.56
1:A:89:TYR:HB3	3:A:410:GOL:H2	1.89	0.54
1:B:87:HIS:HE1	1:B:92:LYS:O	1.91	0.54
1:B:130:CYS:SG	2:B:401[B]:W7B:CAO	2.97	0.53
3:B:406:GOL:H11	6:B:800:HOH:O	2.10	0.52
1:B:5:ASN:CB	6:B:697:HOH:O	2.50	0.51
1:A:5:ASN:OD1	1:A:10:VAL:HG22	2.10	0.50
1:A:9:HIS:HE1	3:A:410:GOL:C1	2.24	0.50
1:B:312:GLU:C	1:B:312:GLU:CD	2.79	0.49
1:B:151:GLN:NE2	6:B:799:HOH:O	2.45	0.49
1:B:99:SER:OG	2:B:401[B]:W7B:H14	2.12	0.49
3:A:410:GOL:H12	6:A:543:HOH:O	2.12	0.49
1:B:46:THR:HG23	1:B:71:LEU:CD2	2.43	0.48
1:B:58:TYR:CD2	3:B:405:GOL:H12	2.48	0.48
1:B:101:LEU:HD12	6:B:856:HOH:O	2.14	0.47
1:A:234:ASN:ND2	1:A:238:ARG:HE	2.05	0.46
1:A:101:LEU:HD22	6:A:828:HOH:O	2.16	0.46
1:B:234:ASN:ND2	1:B:238:ARG:HE	2.09	0.45
3:A:403:GOL:H12	1:B:217:PHE:CE1	2.51	0.45
1:A:226:LEU:HB3	1:A:227:PRO:HD3	1.98	0.45
1:B:99:SER:O	2:B:401[B]:W7B:H13	2.18	0.44
1:B:101:LEU:HD21	2:B:401[B]:W7B:CAQ	2.48	0.44
1:A:59:MET:HE3	1:A:59:MET:HB3	1.79	0.44
1:A:147:ARG:O	1:A:151:GLN:HG3	2.18	0.43
1:B:9:HIS:HE1	6:B:632:HOH:O	2.01	0.43
1:B:188:LYS:HD2	6:B:846:HOH:O	2.17	0.43
1:A:129:SER:HA	1:A:138:GLN:NE2	2.35	0.42
1:A:107:VAL:O	1:A:111:ARG:HG3	2.20	0.41
1:A:44:SER:HB2	1:A:71:LEU:HD11	2.01	0.41
1:A:169:PHE:HD2	3:B:408:GOL:H12	1.85	0.41
1:A:141:TYR:CE2	3:B:408:GOL:H31	2.56	0.41
1:A:143:PHE:CE2	3:A:412:GOL:C3	3.04	0.41
1:A:299:ARG:HD2	6:A:811:HOH:O	2.20	0.40
1:B:0:MET:HE1	1:B:294:ALA:HB2	2.04	0.40
1:B:119:GLU:OE2	6:B:850:HOH:O	2.21	0.40
1:A:13:ASN:HB2	1:A:14:PRO:HD2	2.04	0.40
1:A:53:ASN:HB3	1:A:213:PRO:HG3	2.04	0.40
1:B:97:SER:HA	1:B:125:GLU:O	2.21	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%)	304 (98%)	7 (2%)	0	100	100
1	B	311/313 (99%)	300 (96%)	11 (4%)	0	100	100
All	All	622/626 (99%)	604 (97%)	18 (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%)	256 (99%)	2 (1%)	73	56
1	B	258/258 (100%)	255 (99%)	3 (1%)	63	40
All	All	516/516 (100%)	511 (99%)	5 (1%)	68	47

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LYS
1	A	312	GLU
1	B	5	ASN
1	B	81	LYS
1	B	129	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

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

25 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	405	-	5,5,5	0.78	0	5,5,5	0.70	0
2	W7B	B	401[B]	-	25,25,25	1.61	4 (16%)	33,35,35	1.19	4 (12%)
3	GOL	B	407	-	5,5,5	0.74	0	5,5,5	0.80	0
3	GOL	A	413	-	5,5,5	1.88	1 (20%)	5,5,5	4.17	3 (60%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	GOL	B	402	-	5,5,5	0.66	0	5,5,5	2.66	3 (60%)
3	GOL	B	408	-	5,5,5	3.37	4 (80%)	5,5,5	3.98	4 (80%)
3	GOL	B	406	-	5,5,5	0.91	0	5,5,5	1.07	0
4	FMN	A	414	-	33,33,33	1.79	9 (27%)	48,50,50	1.42	8 (16%)
3	GOL	A	403	-	5,5,5	1.18	1 (20%)	5,5,5	0.90	0
3	GOL	A	404	-	5,5,5	0.98	0	5,5,5	1.38	2 (40%)
3	GOL	B	405	-	5,5,5	0.44	0	5,5,5	0.93	0
3	GOL	B	404	-	5,5,5	0.91	0	5,5,5	1.10	0
5	NCO	B	410	-	6,6,6	3.16	5 (83%)	-		
3	GOL	A	411	-	5,5,5	0.33	0	5,5,5	0.58	0
3	GOL	A	407	-	5,5,5	0.60	0	5,5,5	0.86	0
3	GOL	A	402	-	5,5,5	0.78	0	5,5,5	0.32	0
2	W7B	B	401[A]	-	25,25,25	1.47	5 (20%)	33,35,35	1.90	11 (33%)
3	GOL	A	408	-	5,5,5	0.88	0	5,5,5	0.90	0
3	GOL	A	409	-	5,5,5	0.48	0	5,5,5	1.46	1 (20%)
3	GOL	A	406	-	5,5,5	0.50	0	5,5,5	0.82	0
3	GOL	A	412	-	5,5,5	0.71	0	5,5,5	1.02	0
3	GOL	A	410	-	5,5,5	0.65	0	5,5,5	0.83	0
2	W7B	A	401	-	25,25,25	1.70	8 (32%)	33,35,35	1.79	11 (33%)
4	FMN	B	409	-	33,33,33	1.38	6 (18%)	48,50,50	1.45	7 (14%)
3	GOL	B	403	-	5,5,5	0.67	0	5,5,5	0.81	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
3	GOL	A	405	-	-	4/4/4/4	-
2	W7B	B	401[B]	-	-	3/9/9/9	0/3/3/3
3	GOL	B	407	-	-	0/4/4/4	-
3	GOL	A	413	-	-	2/4/4/4	-
3	GOL	B	402	-	-	1/4/4/4	-
3	GOL	B	408	-	-	1/4/4/4	-
3	GOL	B	406	-	-	4/4/4/4	-
4	FMN	A	414	-	-	1/18/18/18	0/3/3/3
3	GOL	A	403	-	-	0/4/4/4	-
3	GOL	A	404	-	-	0/4/4/4	-
3	GOL	B	405	-	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	B	404	-	-	0/4/4/4	-
3	GOL	A	411	-	-	2/4/4/4	-
3	GOL	A	407	-	-	0/4/4/4	-
3	GOL	A	402	-	-	0/4/4/4	-
2	W7B	B	401[A]	-	-	5/9/9/9	0/3/3/3
3	GOL	A	408	-	-	0/4/4/4	-
3	GOL	A	409	-	-	2/4/4/4	-
3	GOL	A	406	-	-	0/4/4/4	-
3	GOL	A	412	-	-	0/4/4/4	-
3	GOL	A	410	-	-	2/4/4/4	-
2	W7B	A	401	-	-	3/9/9/9	0/3/3/3
4	FMN	B	409	-	-	2/18/18/18	0/3/3/3
3	GOL	B	403	-	-	0/4/4/4	-

All (43) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	414	FMN	C4-N3	-5.22	1.29	1.38
2	B	401[A]	W7B	CAL-C5	-4.55	1.39	1.51
5	B	410	NCO	CO-N6	4.25	2.10	1.96
3	B	408	GOL	O3-C3	4.13	1.59	1.42
3	B	408	GOL	C1-C2	4.12	1.67	1.51
4	A	414	FMN	C5A-N5	-4.08	1.31	1.39
2	B	401[B]	W7B	OAJ-CAI	-3.91	1.19	1.30
2	B	401[B]	W7B	CAL-C5	-3.86	1.41	1.51
5	B	410	NCO	CO-N2	3.71	2.08	1.96
4	A	414	FMN	C5'-C4'	3.63	1.56	1.51
3	B	408	GOL	O1-C1	3.62	1.57	1.42
5	B	410	NCO	CO-N1	3.45	2.07	1.96
3	A	413	GOL	O1-C1	-3.44	1.28	1.42
5	B	410	NCO	CO-N4	3.25	2.07	1.96
2	A	401	W7B	C2-N1	-3.18	1.32	1.37
3	B	408	GOL	C3-C2	3.08	1.63	1.51
4	B	409	FMN	C9-C8	-3.02	1.35	1.39
4	B	409	FMN	O4-C4	3.02	1.29	1.23
4	B	409	FMN	C5A-N5	-2.79	1.34	1.39
4	B	409	FMN	C9A-C5A	2.70	1.45	1.41
2	A	401	W7B	C2-N3	2.56	1.41	1.37
4	B	409	FMN	C4-N3	-2.46	1.34	1.38
2	A	401	W7B	CAT-CAU	2.44	1.41	1.36
2	B	401[A]	W7B	OAJ-CAI	-2.42	1.24	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	414	FMN	C6-C7	-2.37	1.36	1.39
2	A	401	W7B	OAJ-CAI	-2.33	1.24	1.30
2	B	401[B]	W7B	C2-N3	2.32	1.41	1.37
5	B	410	NCO	CO-N3	2.32	2.04	1.96
2	A	401	W7B	C4-CAI	2.30	1.51	1.48
4	A	414	FMN	O4-C4	2.29	1.27	1.23
4	B	409	FMN	C5'-C4'	2.26	1.54	1.51
2	A	401	W7B	C4-N3	2.25	1.43	1.38
2	B	401[A]	W7B	CAT-CAU	2.25	1.41	1.36
2	B	401[A]	W7B	CAP-CAO	2.22	1.42	1.38
2	A	401	W7B	CAU-CAS	-2.21	1.37	1.42
3	A	403	GOL	O3-C3	2.19	1.51	1.42
4	A	414	FMN	C1'-C2'	-2.16	1.49	1.52
4	A	414	FMN	C8M-C8	-2.11	1.47	1.51
4	A	414	FMN	C9A-C5A	2.10	1.44	1.41
2	B	401[B]	W7B	CAP-CAO	2.08	1.42	1.38
2	A	401	W7B	CAO-CAN	2.06	1.41	1.37
2	B	401[A]	W7B	CAM-CAN	-2.05	1.45	1.51
4	A	414	FMN	C6-C5A	-2.05	1.36	1.40

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	413	GOL	C3-C2-C1	-7.62	83.86	111.80
3	B	408	GOL	C3-C2-C1	6.15	134.36	111.80
4	B	409	FMN	C4-C4A-N5	4.43	124.33	118.21
2	B	401[A]	W7B	CAL-C5-C6	4.39	122.52	116.64
3	B	408	GOL	O1-C1-C2	4.23	129.42	110.38
3	B	408	GOL	O3-C3-C2	4.08	128.77	110.38
3	B	402	GOL	O2-C2-C1	-4.02	92.54	109.18
2	A	401	W7B	CAQ-CAP-CAO	-3.98	114.87	121.00
3	A	413	GOL	O3-C3-C2	-3.72	93.65	110.38
4	A	414	FMN	C4-C4A-N5	3.71	123.33	118.21
2	B	401[A]	W7B	CAT-CAW-CAV	3.71	125.36	120.40
3	A	413	GOL	O1-C1-C2	-3.53	94.49	110.38
4	A	414	FMN	O4-C4-C4A	-3.45	117.42	126.53
2	A	401	W7B	CAP-CAQ-CAR	3.40	125.20	120.48
4	B	409	FMN	O4-C4-C4A	-3.38	117.60	126.53
3	B	402	GOL	C3-C2-C1	3.27	123.79	111.80
2	B	401[A]	W7B	CAQ-CAP-CAO	-3.23	116.02	121.00
2	B	401[A]	W7B	CAO-CAN-CAS	-3.23	114.27	119.06
2	B	401[A]	W7B	CAP-CAO-CAN	3.13	127.04	121.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	401	W7B	OAK-CAI-C4	-3.10	114.80	120.20
2	B	401[B]	W7B	O6-C6-C5	-3.05	120.81	124.56
4	B	409	FMN	C6-C5A-N5	3.03	123.48	118.44
4	A	414	FMN	C4A-C4-N3	2.99	120.87	113.25
2	A	401	W7B	C5-C6-N1	2.97	117.96	115.70
2	B	401[A]	W7B	CAQ-CAR-CAS	2.91	122.88	119.12
2	B	401[B]	W7B	C5-C6-N1	2.90	117.91	115.70
4	B	409	FMN	C5A-N5-C4A	2.84	122.69	118.09
2	B	401[B]	W7B	CAN-CAS-CAR	2.75	122.48	119.01
4	B	409	FMN	C9A-C5A-N5	-2.70	119.58	122.45
2	A	401	W7B	OAJ-CAI-OAK	2.69	130.30	123.90
4	A	414	FMN	C5A-C9A-N10	2.55	120.28	117.97
2	B	401[A]	W7B	CAW-CAT-CAU	-2.52	117.02	120.40
2	B	401[A]	W7B	CAQ-CAR-CAV	-2.52	117.26	123.01
3	B	408	GOL	O2-C2-C3	-2.50	98.83	109.18
2	A	401	W7B	OAJ-CAI-C4	-2.47	112.83	116.73
2	A	401	W7B	CAU-CAS-CAR	2.41	121.04	117.92
2	A	401	W7B	N1-C2-N3	2.41	119.53	115.74
4	B	409	FMN	C10-C4A-N5	-2.38	119.95	124.81
2	B	401[B]	W7B	CAL-C5-C4	2.38	124.29	119.56
4	B	409	FMN	C4A-C4-N3	2.37	119.30	113.25
2	A	401	W7B	CAL-C5-C6	2.34	119.78	116.64
3	A	409	GOL	C3-C2-C1	-2.31	103.32	111.80
2	B	401[A]	W7B	CAW-CAV-CAR	-2.31	117.28	120.48
2	B	401[A]	W7B	CAU-CAS-CAR	2.31	120.90	117.92
2	A	401	W7B	O2-C2-N3	-2.29	117.80	121.86
2	A	401	W7B	C6-N1-C2	-2.29	123.22	126.37
4	A	414	FMN	C5A-C6-C7	2.27	125.04	120.83
3	B	402	GOL	O2-C2-C3	-2.27	99.79	109.18
3	A	404	GOL	O1-C1-C2	2.24	120.46	110.38
2	B	401[A]	W7B	C5-C6-N1	2.21	117.38	115.70
4	A	414	FMN	C6-C5A-N5	2.12	121.97	118.44
4	A	414	FMN	C9A-C5A-N5	-2.12	120.20	122.45
4	A	414	FMN	C4-C4A-C10	-2.05	113.41	116.93
3	A	404	GOL	C3-C2-C1	-2.03	104.35	111.80

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	W7B	N3-C4-CAI-OAJ
2	B	401[A]	W7B	N3-C4-CAI-OAJ

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Mol	Chain	Res	Type	Atoms
2	B	401[B]	W7B	N3-C4-CAI-OAJ
2	B	401[B]	W7B	C5-C4-CAI-OAK
3	A	405	GOL	O1-C1-C2-O2
3	A	405	GOL	O1-C1-C2-C3
3	A	405	GOL	C1-C2-C3-O3
3	A	405	GOL	O2-C2-C3-O3
3	A	410	GOL	C1-C2-C3-O3
3	A	413	GOL	C1-C2-C3-O3
3	B	406	GOL	C1-C2-C3-O3
3	B	406	GOL	O2-C2-C3-O3
3	A	410	GOL	O2-C2-C3-O3
3	A	409	GOL	O1-C1-C2-C3
3	B	406	GOL	O1-C1-C2-C3
3	B	402	GOL	O2-C2-C3-O3
3	A	413	GOL	O2-C2-C3-O3
3	B	406	GOL	O1-C1-C2-O2
2	B	401[A]	W7B	C5-CAL-CAM-CAN
3	A	411	GOL	O2-C2-C3-O3
3	B	408	GOL	O1-C1-C2-O2
2	A	401	W7B	C5-C4-CAI-OAK
4	A	414	FMN	C4'-C5'-O5'-P
4	B	409	FMN	C4'-C5'-O5'-P
3	A	411	GOL	C1-C2-C3-O3
2	B	401[B]	W7B	C5-CAL-CAM-CAN
3	A	409	GOL	O1-C1-C2-O2
2	A	401	W7B	C5-C4-CAI-OAJ
2	B	401[A]	W7B	C5-C4-CAI-OAJ
2	B	401[A]	W7B	C5-C4-CAI-OAK
2	B	401[A]	W7B	N3-C4-CAI-OAK
4	B	409	FMN	O3'-C3'-C4'-C5'

There are no ring outliers.

8 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	405	GOL	1	0
2	B	401[B]	W7B	6	0
3	B	408	GOL	3	0
3	B	406	GOL	1	0
3	A	403	GOL	1	0
3	B	405	GOL	1	0
3	A	412	GOL	3	0

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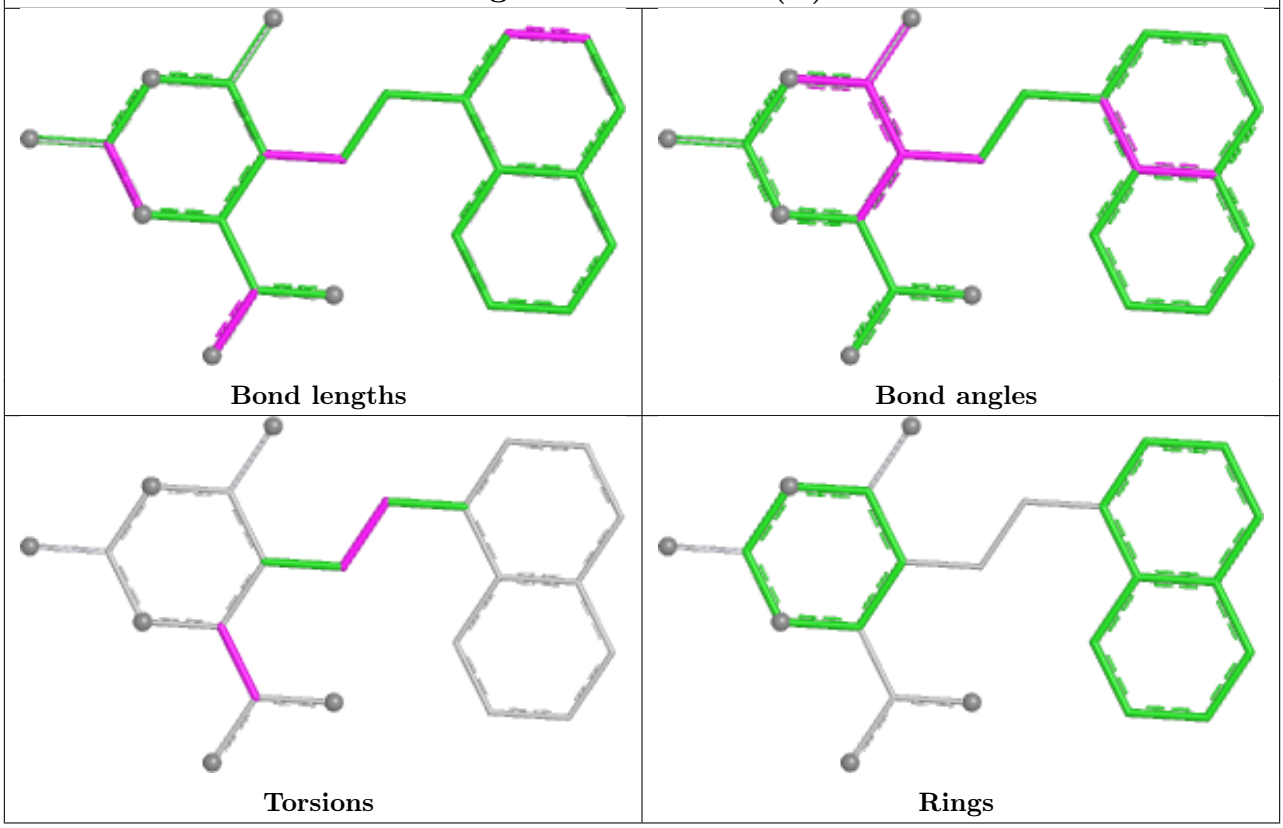
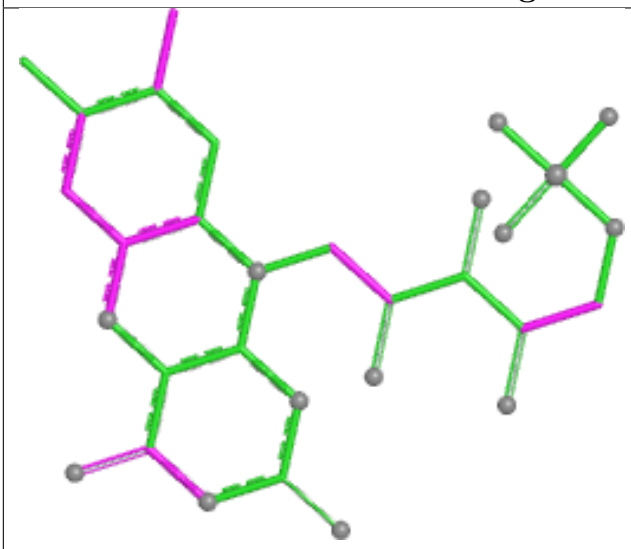
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	410	GOL	7	0

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.

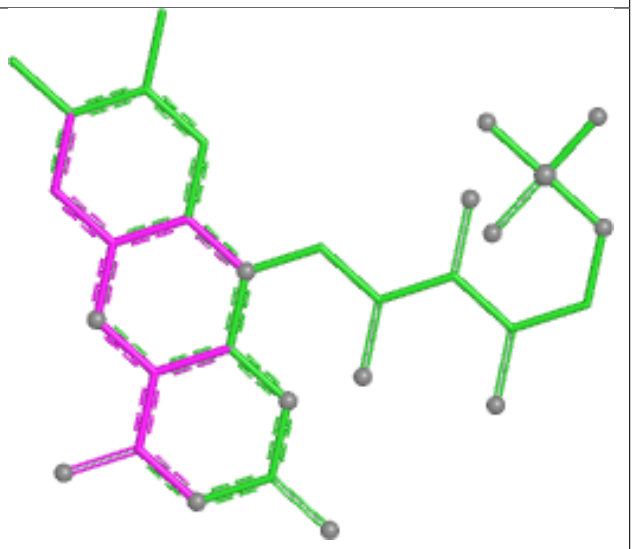
Ligand W7B B 401 (B)



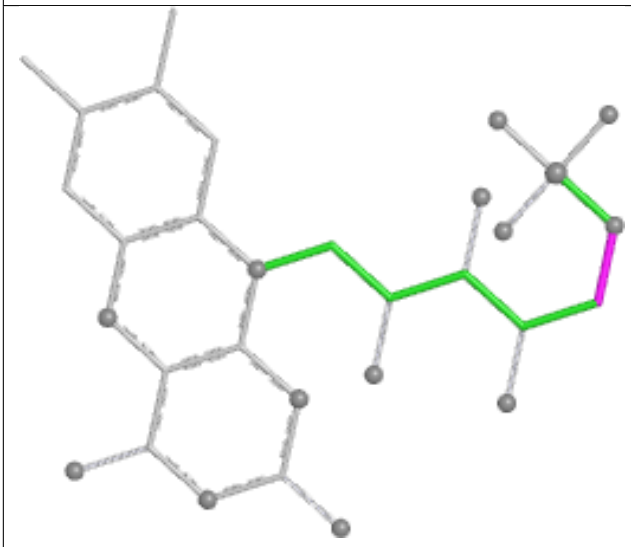
Ligand FMN A 414



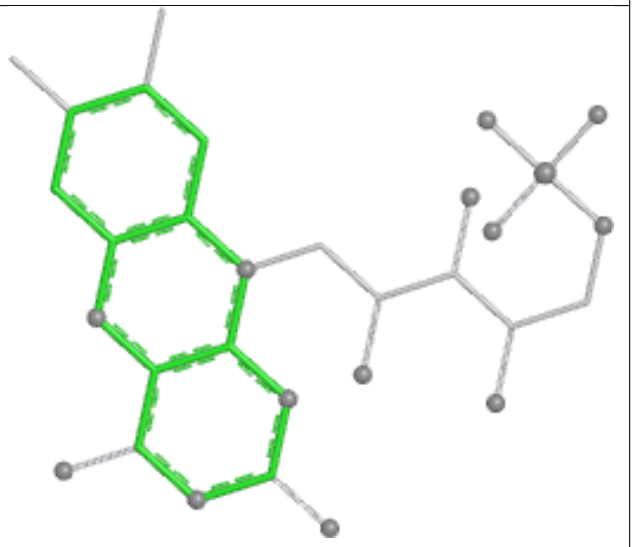
Bond lengths



Bond angles

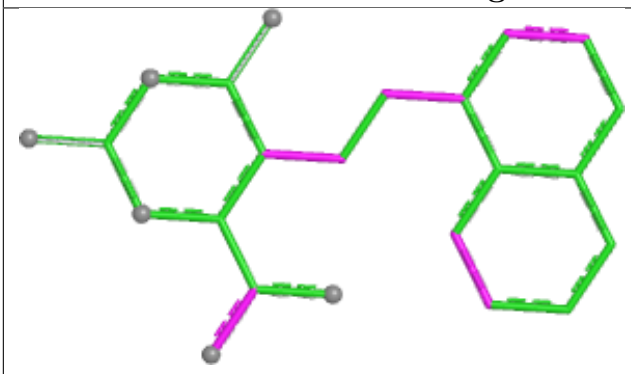


Torsions

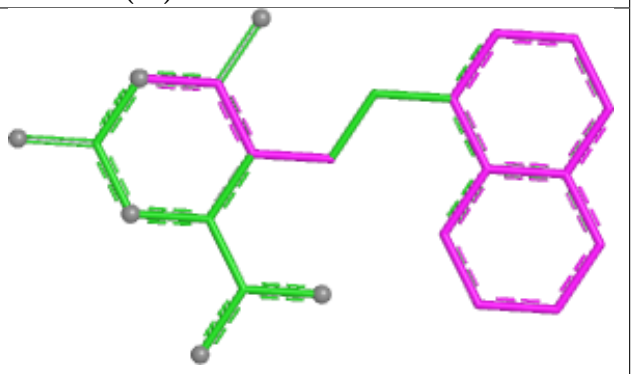


Rings

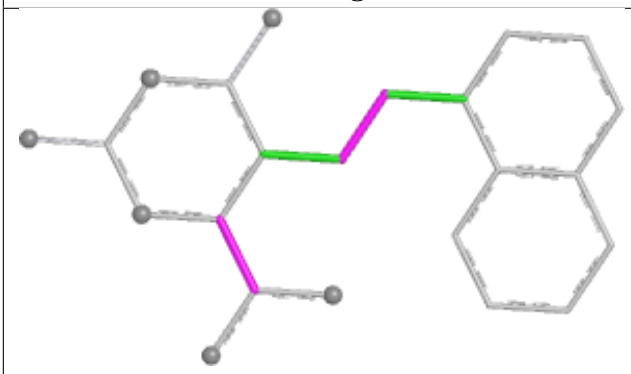
Ligand W7B B 401 (A)



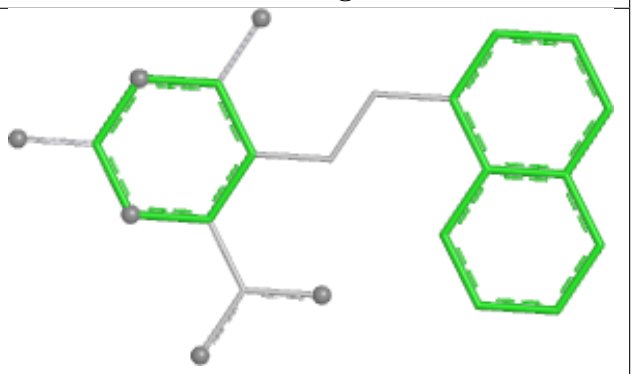
Bond lengths



Bond angles

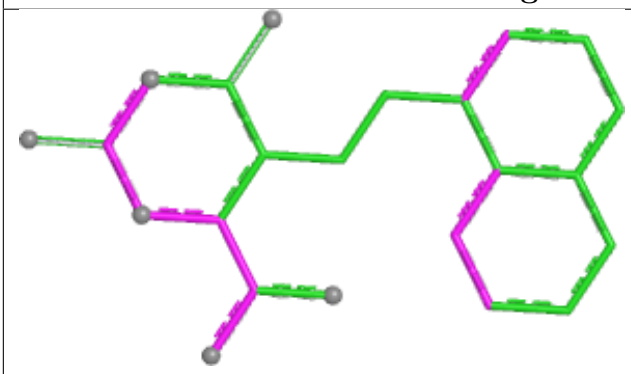


Torsions

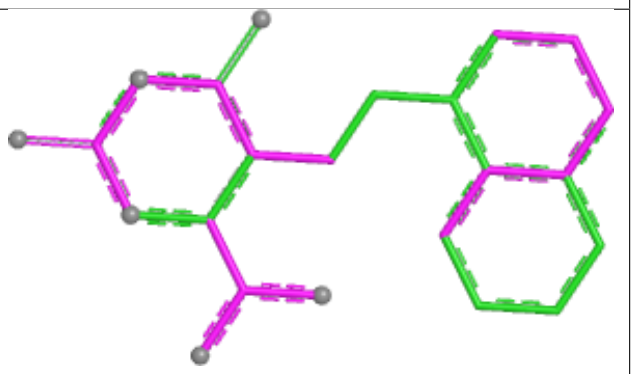


Rings

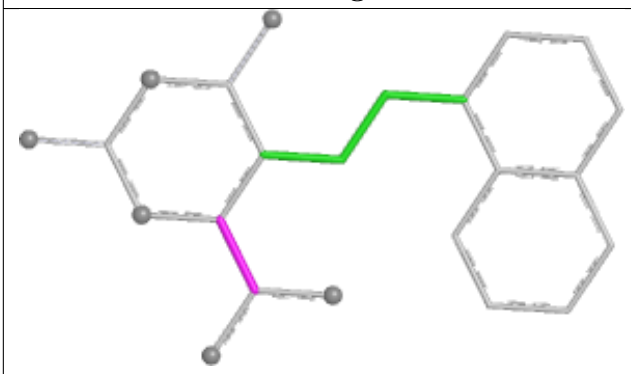
Ligand W7B A 401



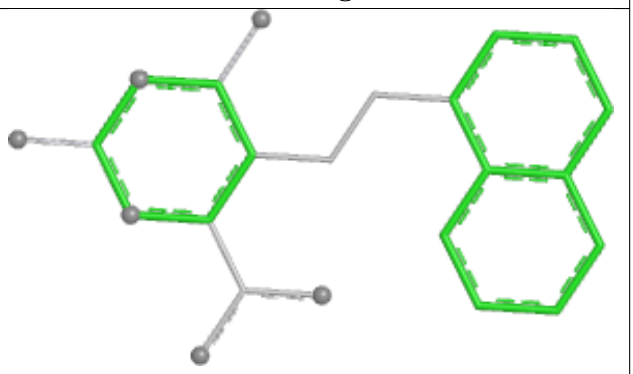
Bond lengths



Bond angles

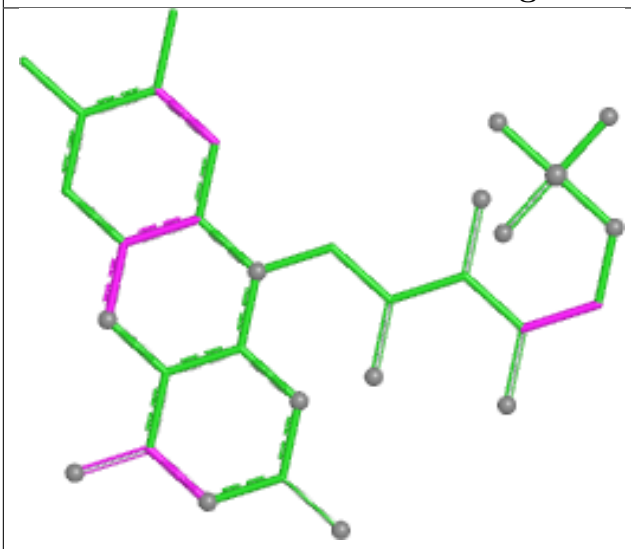


Torsions

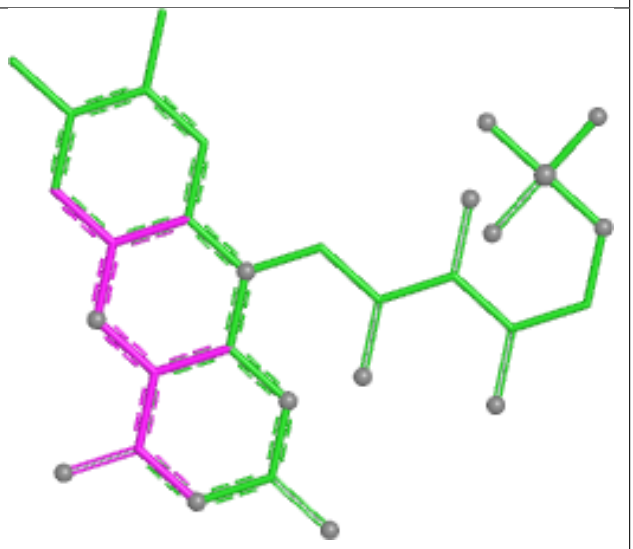


Rings

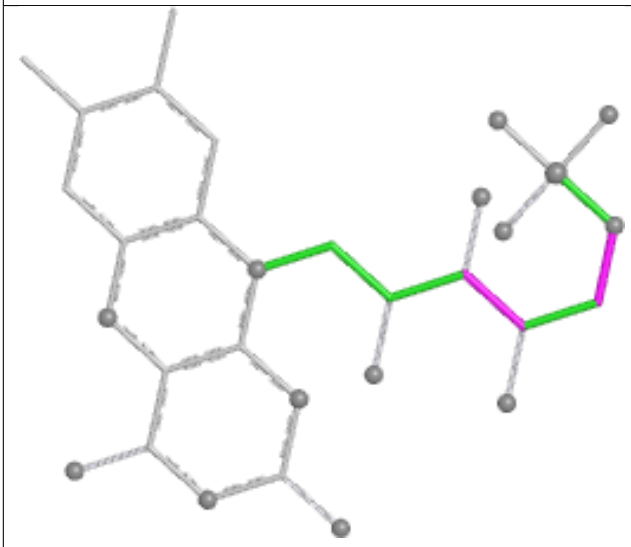
Ligand FMN B 409



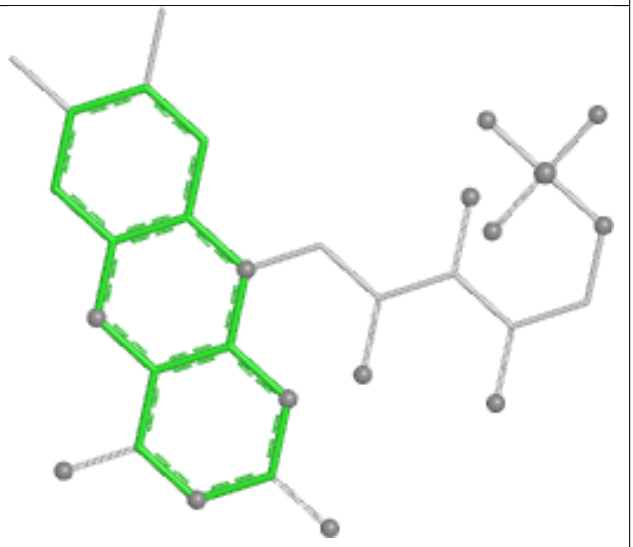
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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%)	-0.24	2 (0%)	85	89	8, 13, 26, 47	0
1	B	313/313 (100%)	-0.32	4 (1%)	75	82	7, 12, 24, 55	0
All	All	626/626 (100%)	-0.28	6 (0%)	79	85	7, 12, 25, 55	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	130	CYS	3.6
1	B	129	SER	3.5
1	A	5	ASN	2.9
1	A	0	MET	2.8
1	B	312	GLU	2.2
1	B	0	MET	2.0

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

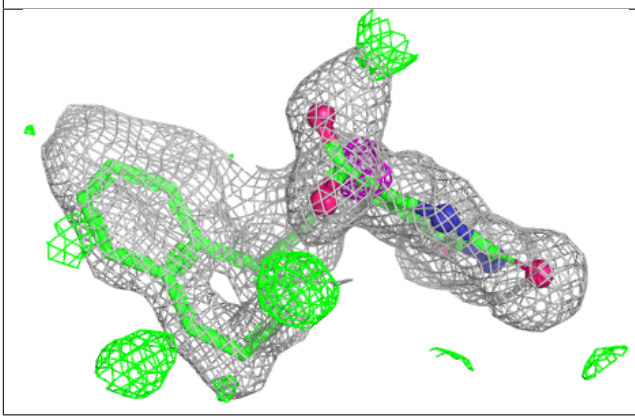
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

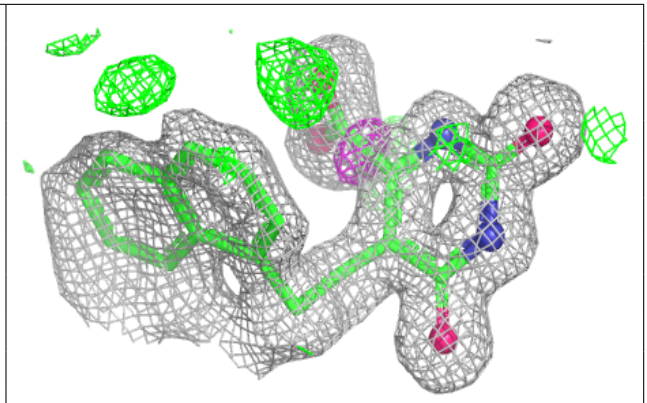
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	GOL	B	406	6/6	0.71	0.19	40,55,57,66	0
3	GOL	A	411	6/6	0.79	0.18	51,53,56,60	0
3	GOL	A	406	6/6	0.79	0.15	34,35,43,46	0
3	GOL	B	405	6/6	0.80	0.17	43,50,51,52	0
3	GOL	B	404	6/6	0.82	0.14	32,36,37,39	0
3	GOL	A	405	6/6	0.84	0.12	34,42,44,46	0
3	GOL	A	408	6/6	0.84	0.15	30,36,43,51	0
3	GOL	A	409	6/6	0.86	0.15	24,39,40,45	0
3	GOL	B	407	6/6	0.86	0.12	34,36,37,39	0
3	GOL	A	410	6/6	0.87	0.12	24,38,43,48	0
3	GOL	A	407	6/6	0.87	0.14	29,40,42,42	0
3	GOL	B	403	6/6	0.88	0.11	25,34,34,35	0
3	GOL	A	404	6/6	0.89	0.11	20,24,30,34	0
3	GOL	B	408	6/6	0.89	0.17	17,30,32,41	0
3	GOL	A	412	6/6	0.90	0.09	31,34,38,39	0
3	GOL	B	402	6/6	0.92	0.10	18,20,22,23	0
3	GOL	A	413	6/6	0.93	0.13	15,29,34,40	0
3	GOL	A	403	6/6	0.94	0.07	22,23,25,28	0
2	W7B	B	401[A]	23/23	0.95	0.07	8,10,12,12	23
2	W7B	B	401[B]	23/23	0.95	0.07	9,10,12,13	23
2	W7B	A	401	23/23	0.96	0.06	9,11,15,16	0
3	GOL	A	402	6/6	0.98	0.05	18,18,20,20	0
4	FMN	B	409	31/31	0.98	0.04	7,8,11,13	0
4	FMN	A	414	31/31	0.99	0.04	7,8,11,11	0
5	NCO	B	410	7/7	0.99	0.07	11,12,13,13	0

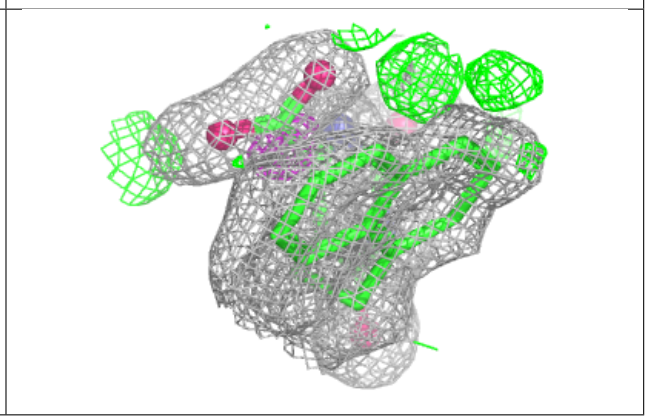
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around W7B B 401 (A):

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

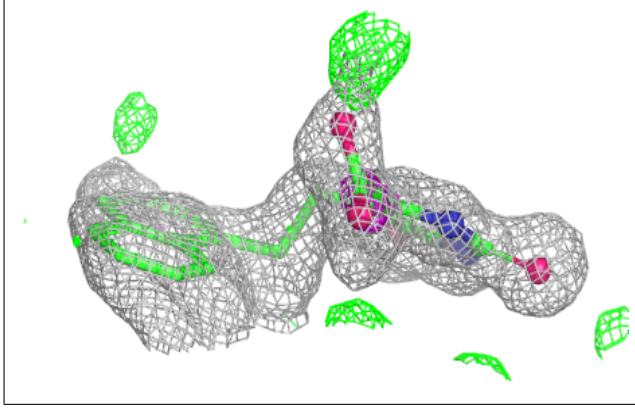


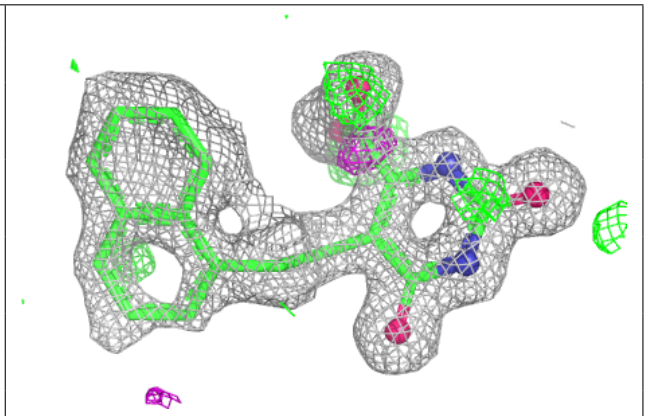


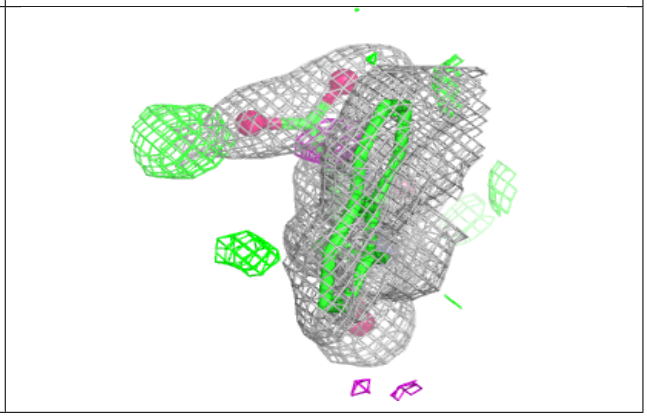


Electron density around W7B B 401 (B):

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

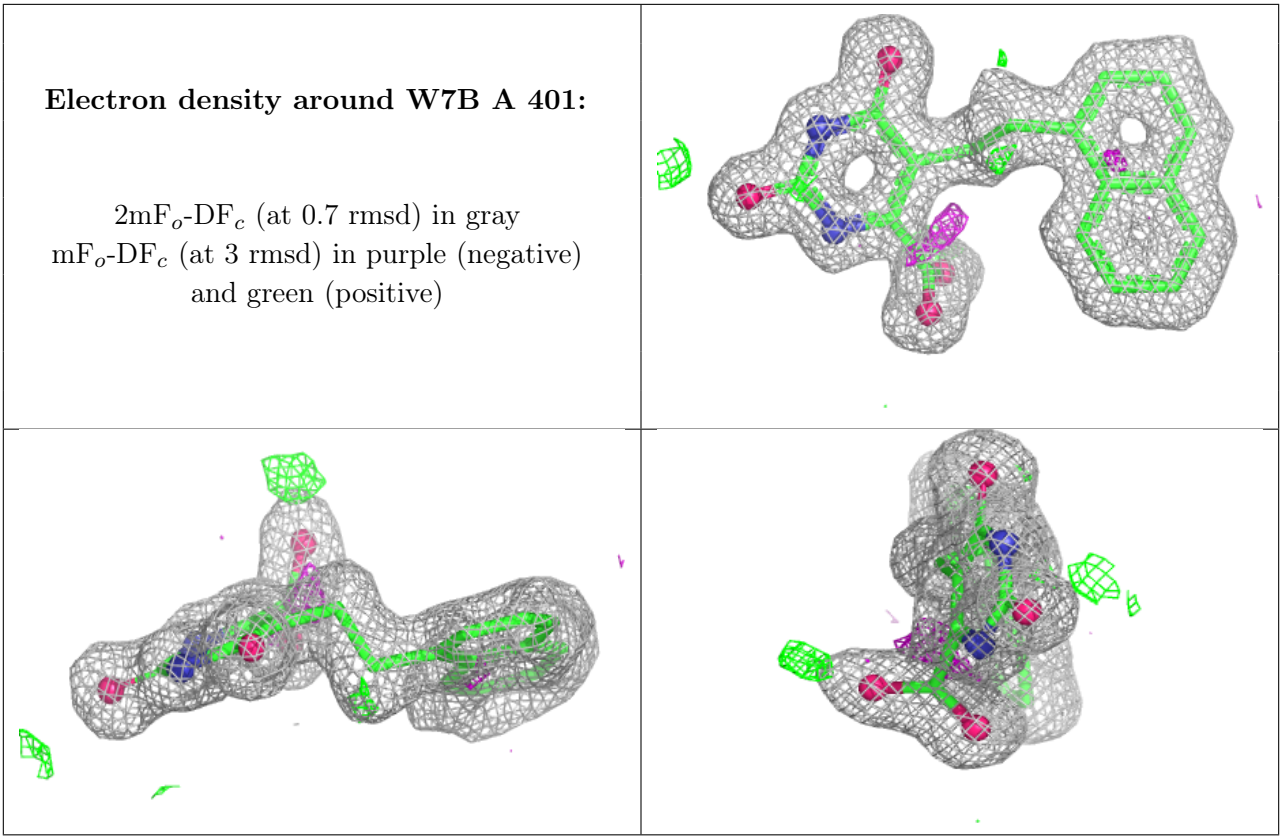






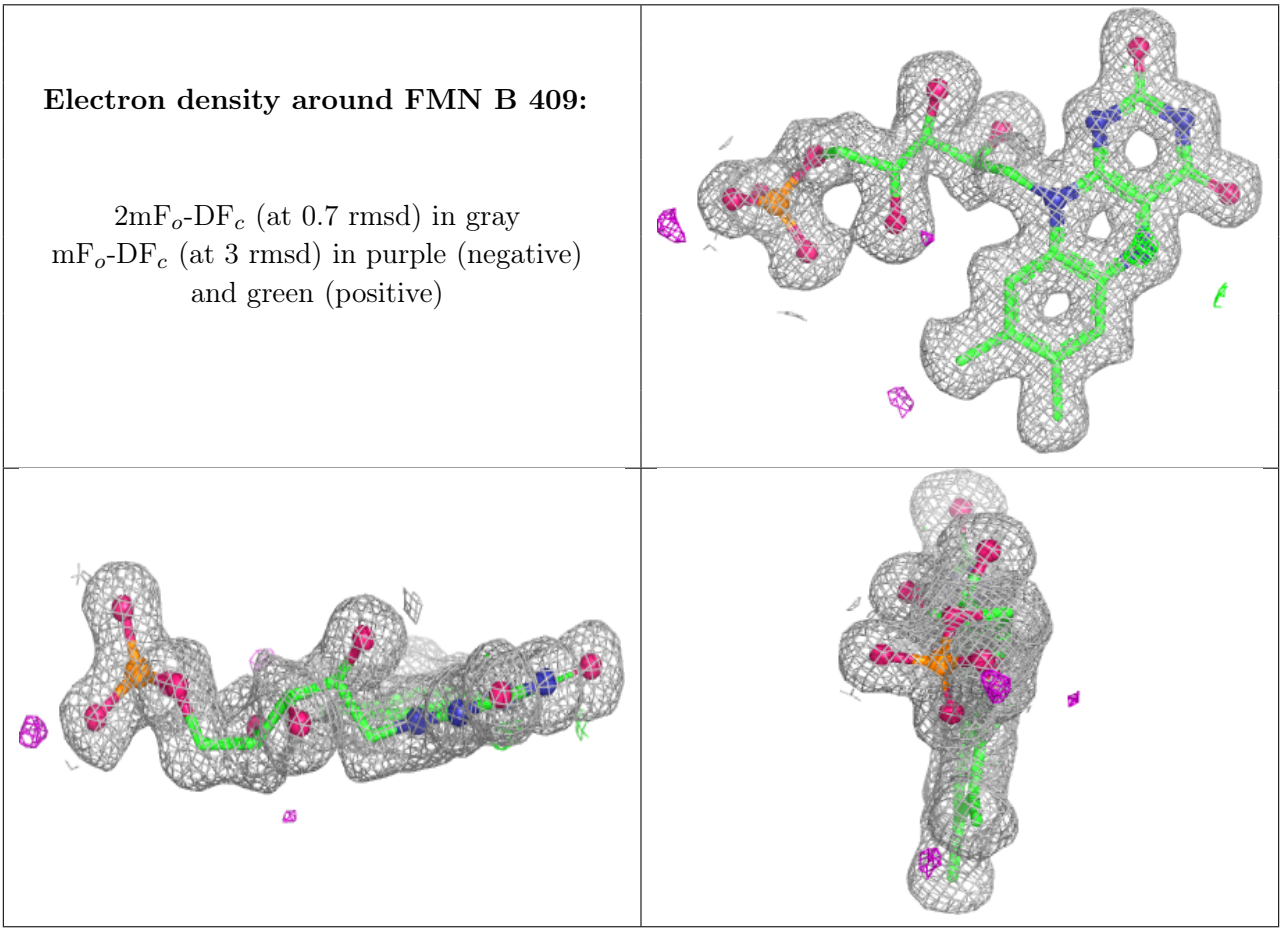
Electron density around W7B A 401:

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



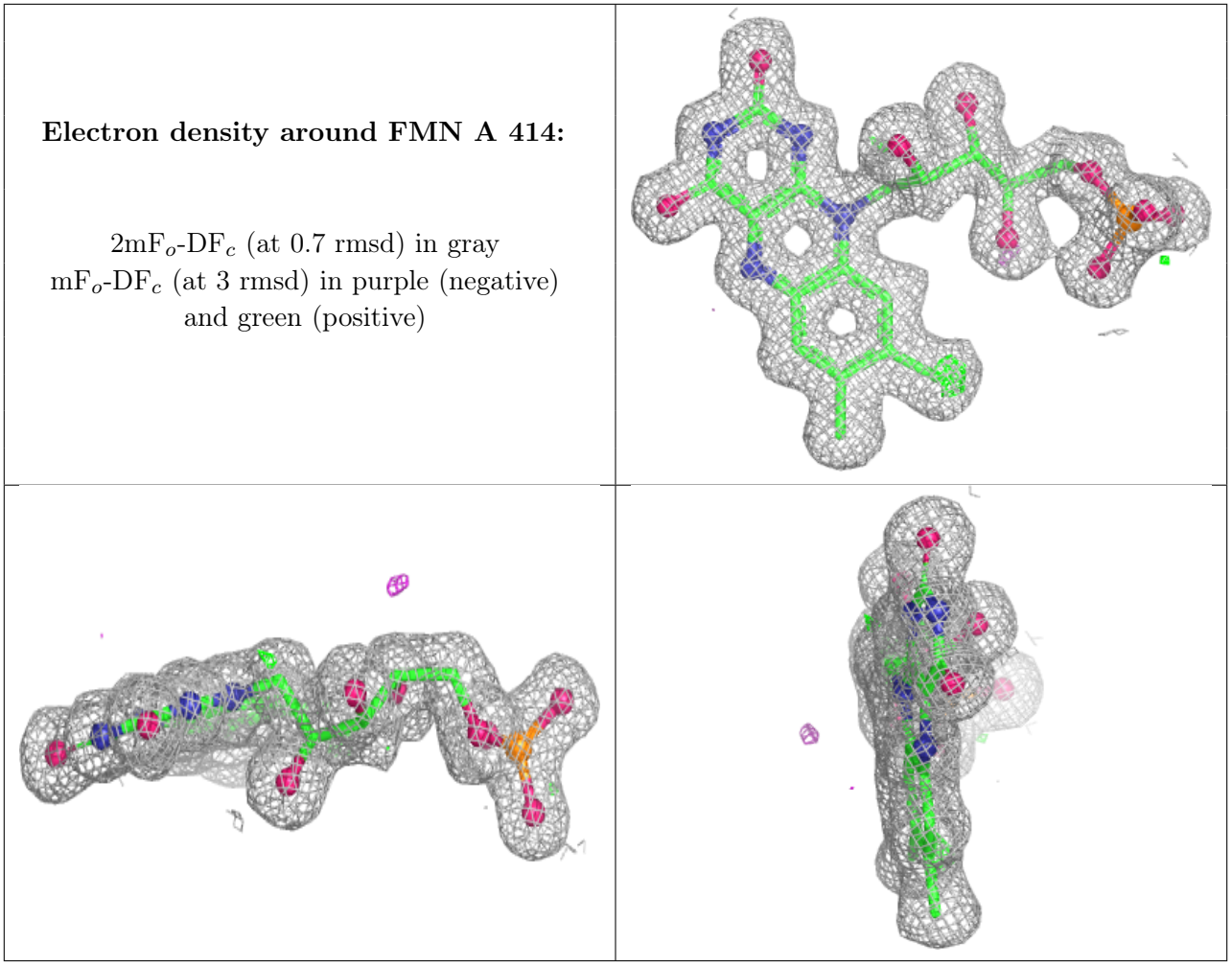
Electron density around FMN B 409:

$2mF_o$-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 414:

$2mF_o$-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.