



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2026 – 08:06 PM EDT

PDB ID : 3W7G / pdb_00003w7g
Title : Structure of Trypanosoma cruzi dihydroorotate dehydrogenase in complex with MII-5-013
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 : 2013-02-28
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 ⓘ 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

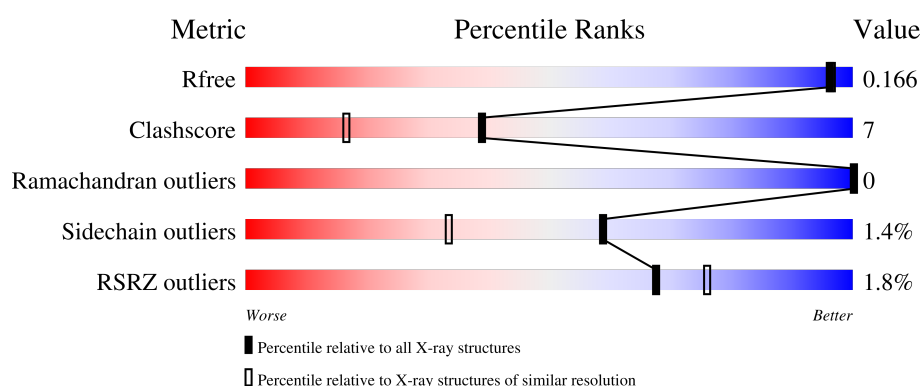
1 Overall quality at a glance

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 $\leq 5\%$. 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	83% 14% .
1	B	313	81% 16% ..

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
2	W7G	B	401[B]	-	-	X	-
3	GOL	B	407	-	-	X	-

2 Entry composition [i](#)

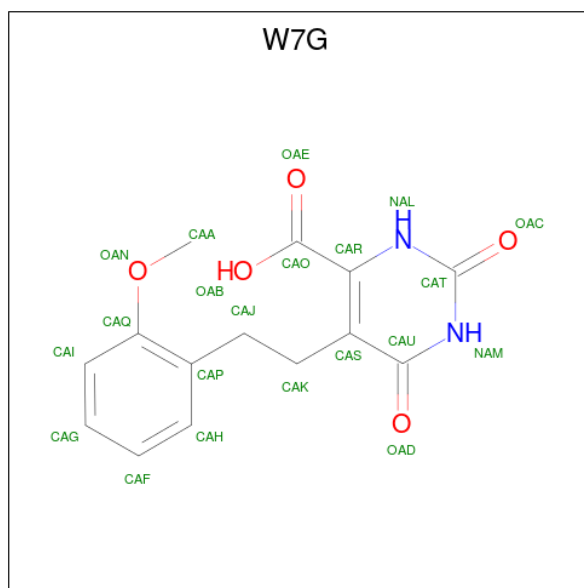
There are 6 unique types of molecules in this entry. The entry contains 5767 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	5	0
			2415	1547	402	448	18			
1	B	313	Total	C	N	O	S	0	3	0
			2402	1539	399	445	19			

- Molecule 2 is 5-[2-(2-methoxyphenyl)ethyl]-2,6-dioxo-1,2,3,6-tetrahydropyrimidine-4-carboxylic acid (CCD ID: W7G) (formula: C₁₄H₁₄N₂O₅).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			21	14	2	5		
2	B	1	Total	C	N	O	0	1
			42	28	4	10		

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	1
			12	6	6		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		

-
- The image displays the chemical structure of Flavin Mononucleotide (FMN). It features an isoalloxazine ring system, which is a tricyclic aromatic heterocycle consisting of a benzene ring fused to two pyrimidine rings. The ring atoms are labeled: N1, N3, N5, N10 for nitrogen atoms and C2, C4, C5A, C6, C7, C8, C9 for carbon atoms. A ribityl chain is attached to the N10 position of the isoalloxazine ring. The ribityl chain consists of three carbon atoms (C1, C2, C3) and a phosphate group. The C1 atom is bonded to a hydroxyl group (OH) and a hydrogen atom (H). The C2 atom is bonded to a hydroxyl group (OH) and a hydrogen atom (H). The C3 atom is bonded to a hydroxyl group (OH) and a hydrogen atom (H). The phosphate group is attached to the C3 atom via an oxygen atom (O5) and consists of a phosphorus atom (P) bonded to four oxygen atoms: one double-bonded (O1P), one single-bonded to a hydroxyl group (OH), and two single-bonded to other oxygen atoms (O2P, O3P).

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

- NCO
-
- The diagram shows a central cobalt atom (Co) in purple, surrounded by six ammonia ligands (NH3) in blue. The ligands are arranged in an octahedral geometry. The top-left ligand is labeled N2, the top-right is N3, the left is N1, the right is N4, the bottom-left is N6, and the bottom-right is N5. A green label 'CO' is placed between the bottom-left and bottom-right ligands. The entire structure is enclosed in a black rectangular box.

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

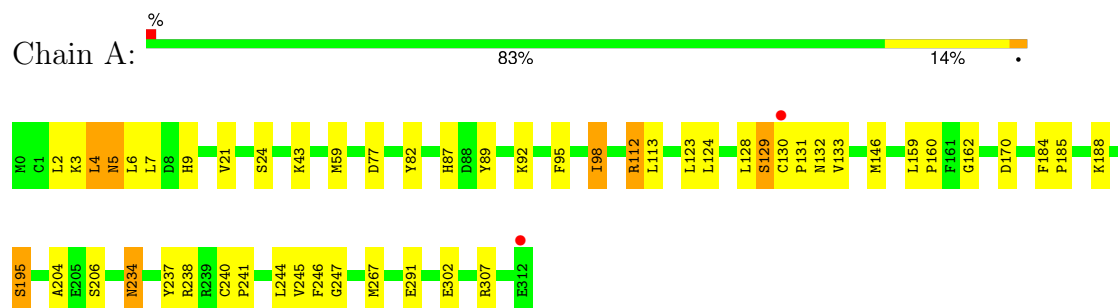
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	374	Total 374	O 374	0	0
6	B	354	Total 354	O 354	0	0

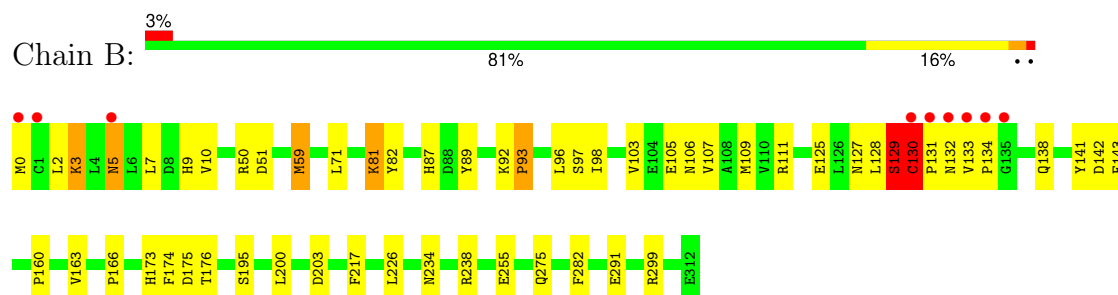
3 Residue-property plots [i](#)

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	67.95Å 71.83Å 129.24Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.88 – 1.55 29.88 – 1.55	Depositor EDS
% Data completeness (in resolution range)	93.0 (29.88-1.55) 92.9 (29.88-1.55)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.79 (at 1.55Å)	Xtrriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.137 , 0.165 0.138 , 0.166	Depositor DCC
R_{free} test set	4295 reflections (4.65%)	wwPDB-VP
Wilson B-factor (Å ²)	11.5	Xtrriage
Anisotropy	0.017	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 43.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	5767	wwPDB-VP
Average B, all atoms (Å ²)	14.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 25.53 % 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 3.1173e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, W7G, NCO, 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	1.61	35/2482 (1.4%)	1.29	5/3360 (0.1%)
1	B	1.61	28/2463 (1.1%)	1.30	8/3336 (0.2%)
All	All	1.61	63/4945 (1.3%)	1.29	13/6696 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	1
All	All	0	3

All (63) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	146	MET	SD-CE	-11.12	1.51	1.79
1	A	21	VAL	C-O	-10.88	1.12	1.24
1	A	246	PHE	C-O	-8.63	1.13	1.24
1	A	204	ALA	C-O	-8.57	1.14	1.24
1	A	129[A]	SER	C-O	-8.55	1.12	1.23
1	A	129[B]	SER	C-O	-8.55	1.12	1.23
1	A	4	LEU	C-O	-8.15	1.13	1.23
1	B	203	ASP	C-O	-7.95	1.14	1.24
1	A	113	LEU	C-O	-7.83	1.14	1.24
1	B	175	ASP	C-O	-7.39	1.15	1.24
1	B	51	ASP	C-O	-7.25	1.15	1.24
1	A	112	ARG	C-O	-7.16	1.14	1.24
1	B	50	ARG	C-O	-7.05	1.15	1.23
1	A	206	SER	C-O	-7.04	1.14	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	5	ASN	CA-C	-7.03	1.44	1.52
1	B	142	ASP	C-O	-7.01	1.16	1.24
1	B	255	GLU	C-O	-6.91	1.15	1.24
1	B	174	PHE	C-O	-6.90	1.16	1.24
1	B	127	ASN	C-O	-6.83	1.15	1.24
1	A	245	VAL	C-O	-6.70	1.17	1.24
1	A	24	SER	C-O	-6.61	1.15	1.24
1	A	240	CYS	CA-C	-6.47	1.44	1.52
1	A	133	VAL	C-O	-6.38	1.15	1.24
1	B	129	SER	C-O	-6.38	1.16	1.23
1	B	134	PRO	C-O	6.18	1.31	1.23
1	B	133	VAL	N-CA	6.15	1.50	1.46
1	A	2	LEU	C-O	-6.09	1.15	1.24
1	A	128	LEU	C-O	-6.08	1.15	1.24
1	B	143	PHE	C-O	-6.04	1.16	1.24
1	A	267	MET	C-O	-6.03	1.16	1.23
1	A	129[A]	SER	N-CA	6.02	1.53	1.46
1	A	129[B]	SER	N-CA	6.02	1.53	1.46
1	B	71	LEU	C-O	5.97	1.26	1.23
1	A	234	ASN	CG-ND2	-5.92	1.20	1.33
1	A	247	GLY	C-O	-5.92	1.15	1.23
1	B	173	HIS	C-O	-5.87	1.17	1.24
1	B	141	TYR	C-O	-5.86	1.16	1.24
1	A	131	PRO	N-CD	5.72	1.55	1.47
1	B	127	ASN	CG-OD1	-5.68	1.12	1.23
1	A	132	ASN	C-O	-5.60	1.17	1.24
1	B	200	LEU	CA-C	-5.49	1.46	1.52
1	A	162	GLY	N-CA	5.35	1.50	1.44
1	A	244	LEU	C-O	-5.35	1.17	1.23
1	B	103	VAL	N-CA	-5.34	1.40	1.46
1	A	234	ASN	CG-OD1	5.33	1.33	1.23
1	A	77	ASP	N-CA	-5.32	1.40	1.46
1	A	131	PRO	C-O	-5.29	1.17	1.23
1	A	98	ILE	C-O	-5.26	1.18	1.24
1	B	282	PHE	C-O	-5.22	1.18	1.24
1	B	160	PRO	CA-CB	-5.20	1.47	1.53
1	B	176	THR	C-O	-5.19	1.18	1.24
1	A	89	TYR	C-O	-5.17	1.17	1.24
1	B	217	PHE	N-CA	5.16	1.52	1.46
1	B	93	PRO	C-O	5.13	1.29	1.23
1	A	130	CYS	C-O	-5.13	1.17	1.24
1	A	195	SER	CA-C	-5.11	1.46	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	59	MET	CA-C	-5.08	1.46	1.52
1	A	6	LEU	CB-CG	-5.08	1.43	1.53
1	B	226	LEU	N-CA	5.08	1.51	1.46
1	A	130	CYS	C-N	5.06	1.40	1.33
1	B	2	LEU	C-N	5.06	1.40	1.33
1	B	106	ASN	C-O	-5.06	1.18	1.24
1	A	5	ASN	C-O	-5.02	1.18	1.24

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	71	LEU	CB-CA-C	6.53	116.85	110.71
1	A	159	LEU	O-C-N	6.25	125.71	121.71
1	B	130[A]	CYS	CA-C-N	-6.22	113.37	119.78
1	B	130[A]	CYS	C-N-CA	-6.22	113.37	119.78
1	B	130[B]	CYS	CA-C-N	-6.22	113.37	119.78
1	B	130[B]	CYS	C-N-CA	-6.22	113.37	119.78
1	A	3	LYS	CD-CE-NZ	5.95	130.92	111.90
1	B	226	LEU	CA-C-N	-5.24	113.64	119.19
1	B	226	LEU	C-N-CA	-5.24	113.64	119.19
1	A	24	SER	N-CA-C	5.10	119.54	112.45
1	A	130	CYS	CA-C-N	-5.04	114.76	119.85
1	A	130	CYS	C-N-CA	-5.04	114.76	119.85
1	B	3	LYS	CA-CB-CG	5.03	124.17	114.10

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	129[A]	SER	Mainchain
1	A	129[B]	SER	Mainchain
1	B	129	SER	Peptide

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	2415	0	2431	18	0
1	B	2402	0	2414	46	0
2	A	21	0	13	0	0
2	B	42	0	26	7	0
3	A	54	0	72	4	0
3	B	36	0	47	10	0
4	A	31	0	19	1	0
4	B	31	0	19	0	0
5	A	7	0	0	0	0
6	A	374	0	0	6	0
6	B	354	0	0	11	0
All	All	5767	0	5041	68	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 7.

All (68) 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:131:PRO:HG3	2:B:401[B]:W7G:CAA	1.74	1.17
1:B:131:PRO:HG3	2:B:401[B]:W7G:H14	1.22	1.09
1:B:132:ASN:HB2	6:B:839:HOH:O	1.61	0.97
1:B:131:PRO:CG	2:B:401[B]:W7G:H14	2.05	0.86
1:B:9:HIS:CE1	3:B:407:GOL:H32	2.11	0.84
1:B:128:LEU:HD12	1:B:163:VAL:CG1	2.12	0.80
1:B:128:LEU:HD12	1:B:163:VAL:HG11	1.63	0.80
1:A:241:PRO:HA	3:A:409:GOL:H32	1.68	0.74
1:B:131:PRO:HG3	2:B:401[B]:W7G:H12	1.69	0.74
1:B:128:LEU:CD1	1:B:163:VAL:HG11	2.19	0.71
1:B:9:HIS:ND1	3:B:407:GOL:H32	2.05	0.71
1:B:96:LEU:CD2	1:B:98:ILE:HD11	2.20	0.70
1:B:131:PRO:CG	2:B:401[B]:W7G:CAA	2.62	0.70
1:B:128:LEU:CD1	1:B:163:VAL:CG1	2.69	0.69
1:B:234:ASN:HD21	1:B:238:ARG:HE	1.38	0.69
1:A:7:LEU:O	1:A:9:HIS:HD2	1.76	0.69
1:A:59:MET:HE3	6:A:624:HOH:O	1.93	0.68
1:B:0:MET:HE1	1:B:299:ARG:HA	1.77	0.66
1:A:234:ASN:HD21	1:A:238:ARG:HE	1.44	0.65
1:A:82:TYR:OH	1:A:87:HIS:HD2	1.82	0.62
1:B:59:MET:HE3	6:B:616:HOH:O	2.00	0.59
1:B:81:LYS:HE3	6:B:737:HOH:O	2.03	0.58
1:B:9:HIS:CE1	3:B:407:GOL:C3	2.84	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:96:LEU:CD2	1:B:98:ILE:CD1	2.84	0.56
1:A:43:LYS:HE3	4:A:410:FMN:O4	2.05	0.56
1:B:81:LYS:CE	6:B:737:HOH:O	2.53	0.56
1:B:82:TYR:OH	1:B:87:HIS:HD2	1.88	0.56
3:B:407:GOL:C3	6:B:510:HOH:O	2.54	0.56
1:A:291:GLU:CD	6:A:770:HOH:O	2.48	0.55
1:B:89:TYR:HB3	3:B:407:GOL:H11	1.88	0.55
1:B:195:SER:HB3	6:B:777:HOH:O	2.08	0.54
3:A:409:GOL:H31	6:A:571:HOH:O	2.09	0.53
1:A:87:HIS:HE1	1:A:92:LYS:O	1.92	0.53
1:B:89:TYR:HD1	3:B:407:GOL:H31	1.73	0.52
1:B:234:ASN:ND2	1:B:238:ARG:HE	2.08	0.51
1:B:107:VAL:O	1:B:111:ARG:HG3	2.11	0.51
1:A:237:TYR:O	3:A:409:GOL:H11	2.12	0.50
1:B:130[B]:CYS:H	1:B:138:GLN:HE22	1.60	0.50
3:B:402:GOL:H12	6:B:699:HOH:O	2.10	0.50
1:B:87:HIS:HE1	1:B:92:LYS:O	1.95	0.49
1:B:130[A]:CYS:H	1:B:138:GLN:HE22	1.61	0.49
3:B:407:GOL:H31	6:B:510:HOH:O	2.12	0.49
1:A:112:ARG:HD3	6:A:873:HOH:O	2.13	0.48
1:B:129:SER:C	1:B:130[B]:CYS:SG	2.93	0.48
1:B:291:GLU:CD	6:B:611:HOH:O	2.57	0.47
1:B:93:PRO:HA	3:B:407:GOL:H12	1.97	0.47
1:B:96:LEU:HD21	1:B:98:ILE:HD11	1.96	0.47
1:B:131:PRO:HD3	2:B:401[B]:W7G:OAN	2.15	0.45
1:B:7:LEU:O	1:B:9:HIS:HD2	1.99	0.45
1:A:170:ASP:OD2	1:B:138:GLN:HG2	2.17	0.45
1:B:128:LEU:CD1	1:B:163:VAL:HG13	2.47	0.45
1:B:5:ASN:OD1	1:B:10:VAL:HG22	2.16	0.44
1:A:302:GLU:OE2	3:A:403:GOL:C3	2.66	0.44
2:B:401[B]:W7G:H14	2:B:401[B]:W7G:H11	1.57	0.43
1:A:160:PRO:HB3	1:A:188:LYS:HG3	2.01	0.43
1:B:97:SER:HA	1:B:125:GLU:O	2.18	0.43
1:B:0:MET:HE2	6:B:800:HOH:O	2.18	0.42
1:A:95:PHE:HA	1:A:123:LEU:O	2.20	0.42
1:B:105:GLU:HG2	1:B:109:MET:HE2	2.00	0.42
1:A:98:ILE:HG12	1:A:124:LEU:HD11	2.02	0.42
1:A:9:HIS:HE1	6:A:526:HOH:O	2.02	0.41
1:B:9:HIS:HE1	3:B:407:GOL:C3	2.34	0.41
1:B:96:LEU:HD22	1:B:98:ILE:HD11	2.00	0.41
1:B:81:LYS:HB2	1:B:81:LYS:HE2	1.90	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:307[B]:ARG:NH2	6:A:859:HOH:O	2.53	0.40
1:B:275:GLN:NE2	6:B:606:HOH:O	2.50	0.40
1:A:184:PHE:HA	1:A:185:PRO:HD2	1.97	0.40
1:B:128:LEU:HD11	1:B:163:VAL:HG11	2.01	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	316/313 (101%)	307 (97%)	9 (3%)	0	100	100
1	B	314/313 (100%)	308 (98%)	6 (2%)	0	100	100
All	All	630/626 (101%)	615 (98%)	15 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	263/258 (102%)	260 (99%)	3 (1%)	65	43
1	B	261/258 (101%)	256 (98%)	5 (2%)	50	22
All	All	524/516 (102%)	516 (98%)	8 (2%)	59	31

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LEU
1	A	5	ASN
1	A	195	SER
1	B	3	LYS
1	B	81	LYS
1	B	130[A]	CYS
1	B	130[B]	CYS
1	B	166	PRO

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

Mol	Chain	Res	Type
1	A	5	ASN
1	A	9	HIS
1	A	87	HIS
1	A	132	ASN
1	A	151	GLN
1	A	234	ASN
1	B	9	HIS
1	B	87	HIS
1	B	138	GLN
1	B	234	ASN
1	B	275	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

21 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$
2	W7G	A	401	-	22,22,22	1.55	6 (27%)	28,30,30	1.47	5 (17%)
3	GOL	B	403	-	5,5,5	1.30	1 (20%)	5,5,5	1.54	2 (40%)
3	GOL	A	409	-	5,5,5	0.48	0	5,5,5	0.87	0
3	GOL	A	404	-	5,5,5	0.89	0	5,5,5	0.91	0
3	GOL	B	405	-	5,5,5	0.70	0	5,5,5	0.33	0
3	GOL	A	406	-	5,5,5	0.30	0	5,5,5	0.48	0
3	GOL	B	407	-	5,5,5	0.79	0	5,5,5	1.80	1 (20%)
4	FMN	A	410	-	33,33,33	1.39	6 (18%)	48,50,50	1.28	6 (12%)
2	W7G	B	401[A]	-	22,22,22	1.70	5 (22%)	28,30,30	1.80	7 (25%)
5	NCO	A	411	-	6,6,6	3.68	6 (100%)	-		
3	GOL	B	404	-	5,5,5	0.40	0	5,5,5	0.47	0
4	FMN	B	408	-	33,33,33	1.39	5 (15%)	48,50,50	1.17	3 (6%)
3	GOL	A	405	-	5,5,5	0.43	0	5,5,5	0.72	0
3	GOL	A	402	-	5,5,5	0.62	0	5,5,5	2.33	4 (80%)
3	GOL	A	407[A]	-	5,5,5	0.69	0	5,5,5	0.61	0
2	W7G	B	401[B]	-	22,22,22	1.71	6 (27%)	28,30,30	2.36	9 (32%)
3	GOL	A	407[B]	-	5,5,5	0.68	0	5,5,5	0.44	0
3	GOL	B	402	-	5,5,5	0.47	0	5,5,5	0.47	0
3	GOL	A	408	-	5,5,5	0.39	0	5,5,5	0.62	0
3	GOL	B	406	-	5,5,5	0.83	0	5,5,5	1.34	0
3	GOL	A	403	-	5,5,5	0.68	0	5,5,5	0.82	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	W7G	A	401	-	-	3/11/11/11	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	B	403	-	-	0/4/4/4	-
3	GOL	A	409	-	-	3/4/4/4	-
3	GOL	A	404	-	-	0/4/4/4	-
3	GOL	B	405	-	-	0/4/4/4	-
3	GOL	A	406	-	-	2/4/4/4	-
3	GOL	B	407	-	-	4/4/4/4	-
4	FMN	A	410	-	-	1/18/18/18	0/3/3/3
2	W7G	B	401[A]	-	-	3/11/11/11	0/2/2/2
3	GOL	B	404	-	-	2/4/4/4	-
4	FMN	B	408	-	-	1/18/18/18	0/3/3/3
3	GOL	A	405	-	-	1/4/4/4	-
3	GOL	A	402	-	-	0/4/4/4	-
3	GOL	A	407[A]	-	-	0/4/4/4	-
2	W7G	B	401[B]	-	-	3/11/11/11	0/2/2/2
3	GOL	A	407[B]	-	-	0/4/4/4	-
3	GOL	B	402	-	-	2/4/4/4	-
3	GOL	A	408	-	-	0/4/4/4	-
3	GOL	B	406	-	-	2/4/4/4	-
3	GOL	A	403	-	-	3/4/4/4	-

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401[B]	W7G	CAJ-CAP	-4.84	1.42	1.51
5	A	411	NCO	CO-N6	4.19	2.10	1.96
5	A	411	NCO	CO-N3	4.13	2.09	1.96
2	B	401[A]	W7G	CAJ-CAP	-4.01	1.44	1.51
5	A	411	NCO	CO-N1	3.98	2.09	1.96
5	A	411	NCO	CO-N5	3.63	2.08	1.96
4	B	408	FMN	O4-C4	3.26	1.29	1.23
5	A	411	NCO	CO-N4	3.09	2.06	1.96
4	A	410	FMN	C5'-C4'	3.07	1.56	1.51
2	B	401[B]	W7G	CAR-CAO	-3.03	1.43	1.48
2	A	401	W7G	CAH-CAP	2.94	1.44	1.39
2	B	401[A]	W7G	OAN-CAA	2.90	1.50	1.42
4	A	410	FMN	C4A-N5	2.89	1.37	1.30
2	A	401	W7G	CAU-CAS	-2.86	1.39	1.44
2	B	401[A]	W7G	CAR-CAO	-2.85	1.43	1.48
4	B	408	FMN	C4-N3	-2.83	1.33	1.38
5	A	411	NCO	CO-N2	2.81	2.05	1.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401[B]	W7G	OAN-CAQ	-2.75	1.32	1.37
2	A	401	W7G	CAJ-CAP	-2.73	1.46	1.51
3	B	403	GOL	O2-C2	2.71	1.51	1.43
2	B	401[B]	W7G	CAF-CAH	2.66	1.43	1.38
4	B	408	FMN	C5A-N5	-2.61	1.34	1.39
2	A	401	W7G	OAN-CAA	2.55	1.50	1.42
4	A	410	FMN	C9A-C5A	2.50	1.45	1.41
4	B	408	FMN	C1'-C2'	-2.42	1.49	1.52
4	A	410	FMN	C2-N3	-2.41	1.33	1.39
4	B	408	FMN	C2'-C3'	-2.29	1.49	1.53
2	B	401[B]	W7G	CAU-CAS	-2.26	1.40	1.44
2	B	401[A]	W7G	OAB-CAO	-2.25	1.24	1.30
2	B	401[B]	W7G	OAB-CAO	-2.25	1.24	1.30
2	A	401	W7G	CAQ-CAP	2.23	1.43	1.39
2	B	401[A]	W7G	CAI-CAQ	2.16	1.44	1.39
4	A	410	FMN	C2'-C3'	-2.09	1.49	1.53
2	A	401	W7G	CAK-CAS	-2.03	1.46	1.51
4	A	410	FMN	C6-C7	-2.00	1.36	1.39

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401[B]	W7G	CAA-OAN-CAQ	-7.50	106.52	117.51
2	B	401[B]	W7G	CAS-CAU-NAM	5.22	119.67	115.70
2	B	401[A]	W7G	CAK-CAS-CAU	4.62	122.83	116.64
2	B	401[B]	W7G	CAU-NAM-CAT	-4.11	120.71	126.37
2	B	401[A]	W7G	CAU-NAM-CAT	-3.73	121.23	126.37
2	B	401[A]	W7G	CAS-CAU-NAM	3.67	118.49	115.70
3	B	407	GOL	C3-C2-C1	-3.49	99.00	111.80
4	A	410	FMN	O2-C2-N1	-3.43	116.11	121.80
2	A	401	W7G	CAH-CAP-CAQ	-3.38	113.75	118.37
4	A	410	FMN	O4-C4-C4A	-3.38	117.60	126.53
4	B	408	FMN	C8M-C8-C7	3.20	127.30	120.76
2	B	401[B]	W7G	OAN-CAQ-CAI	-3.18	118.94	124.30
2	B	401[A]	W7G	OAD-CAU-NAM	-3.10	114.28	120.11
2	A	401	W7G	OAN-CAQ-CAP	-3.02	111.46	115.96
3	A	402	GOL	O2-C2-C1	-2.90	97.16	109.18
2	B	401[B]	W7G	OAD-CAU-NAM	-2.88	114.71	120.11
2	B	401[B]	W7G	CAI-CAQ-CAP	2.84	125.11	120.18
3	A	402	GOL	O2-C2-C3	2.78	120.70	109.18
3	B	403	GOL	O2-C2-C3	2.77	120.63	109.18
4	B	408	FMN	C8M-C8-C9	-2.73	114.76	119.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	W7G	CAO-CAR-CAS	2.57	127.78	123.88
2	A	401	W7G	OAB-CAO-CAR	-2.47	112.82	116.73
4	B	408	FMN	C7M-C7-C8	-2.44	115.78	120.76
4	A	410	FMN	C4A-C4-N3	2.42	119.42	113.25
2	B	401[A]	W7G	OAN-CAQ-CAP	-2.42	112.36	115.96
2	B	401[B]	W7G	NAM-CAT-NAL	2.32	119.39	115.74
2	B	401[A]	W7G	NAM-CAT-NAL	2.30	119.35	115.74
4	A	410	FMN	C4-N3-C2	-2.26	121.63	125.64
2	B	401[B]	W7G	CAH-CAP-CAQ	-2.25	115.30	118.37
3	A	402	GOL	O1-C1-C2	-2.22	100.39	110.38
3	A	402	GOL	C3-C2-C1	-2.21	103.68	111.80
4	A	410	FMN	O5'-C5'-C4'	2.14	115.07	109.36
2	A	401	W7G	CAJ-CAP-CAH	2.13	124.04	119.42
2	B	401[B]	W7G	CAK-CAS-CAR	2.11	123.75	119.56
2	B	401[A]	W7G	OAD-CAU-CAS	2.09	127.14	124.56
4	A	410	FMN	C9A-C5A-N5	-2.08	120.25	122.45
3	B	403	GOL	C3-C2-C1	-2.00	104.45	111.80

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	W7G	OAB-CAO-CAR-NAL
2	B	401[A]	W7G	OAB-CAO-CAR-NAL
2	B	401[B]	W7G	OAB-CAO-CAR-NAL
3	A	403	GOL	O1-C1-C2-C3
3	A	406	GOL	O1-C1-C2-C3
3	A	409	GOL	O1-C1-C2-C3
3	B	402	GOL	C1-C2-C3-O3
3	B	404	GOL	C1-C2-C3-O3
3	B	406	GOL	O1-C1-C2-C3
3	B	407	GOL	O1-C1-C2-C3
3	B	407	GOL	C1-C2-C3-O3
3	A	405	GOL	C1-C2-C3-O3
3	A	406	GOL	O1-C1-C2-O2
3	A	409	GOL	O1-C1-C2-O2
3	B	402	GOL	O2-C2-C3-O3
3	B	406	GOL	O1-C1-C2-O2
3	B	407	GOL	O1-C1-C2-O2
3	B	407	GOL	O2-C2-C3-O3
3	A	403	GOL	O1-C1-C2-O2
3	B	404	GOL	O2-C2-C3-O3

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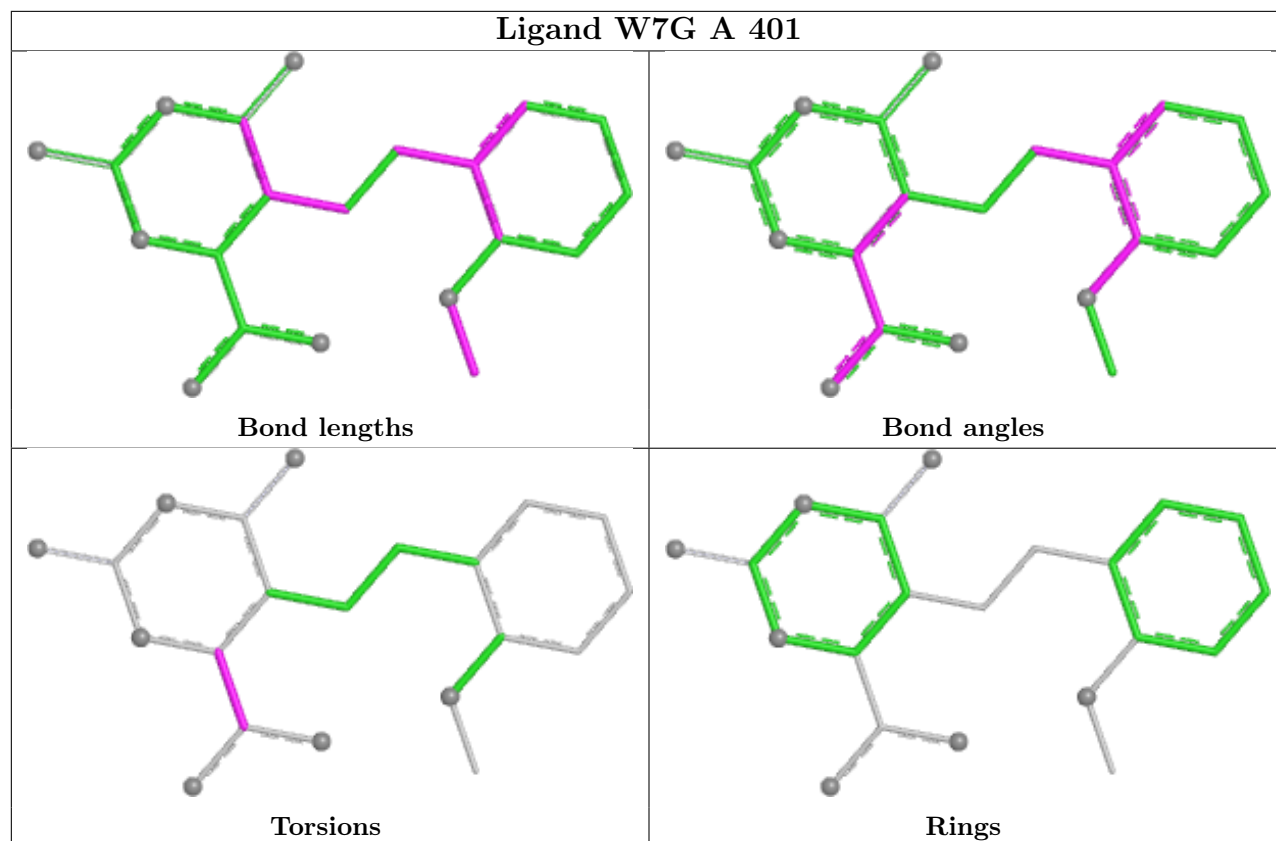
Mol	Chain	Res	Type	Atoms
3	A	409	GOL	O2-C2-C3-O3
4	A	410	FMN	C4'-C5'-O5'-P
2	A	401	W7G	OAE-CAO-CAR-CAS
4	B	408	FMN	C4'-C5'-O5'-P
3	A	403	GOL	O2-C2-C3-O3
2	B	401[A]	W7G	OAE-CAO-CAR-CAS
2	B	401[B]	W7G	OAE-CAO-CAR-CAS
2	A	401	W7G	OAE-CAO-CAR-NAL
2	B	401[A]	W7G	OAE-CAO-CAR-NAL
2	B	401[B]	W7G	OAE-CAO-CAR-NAL

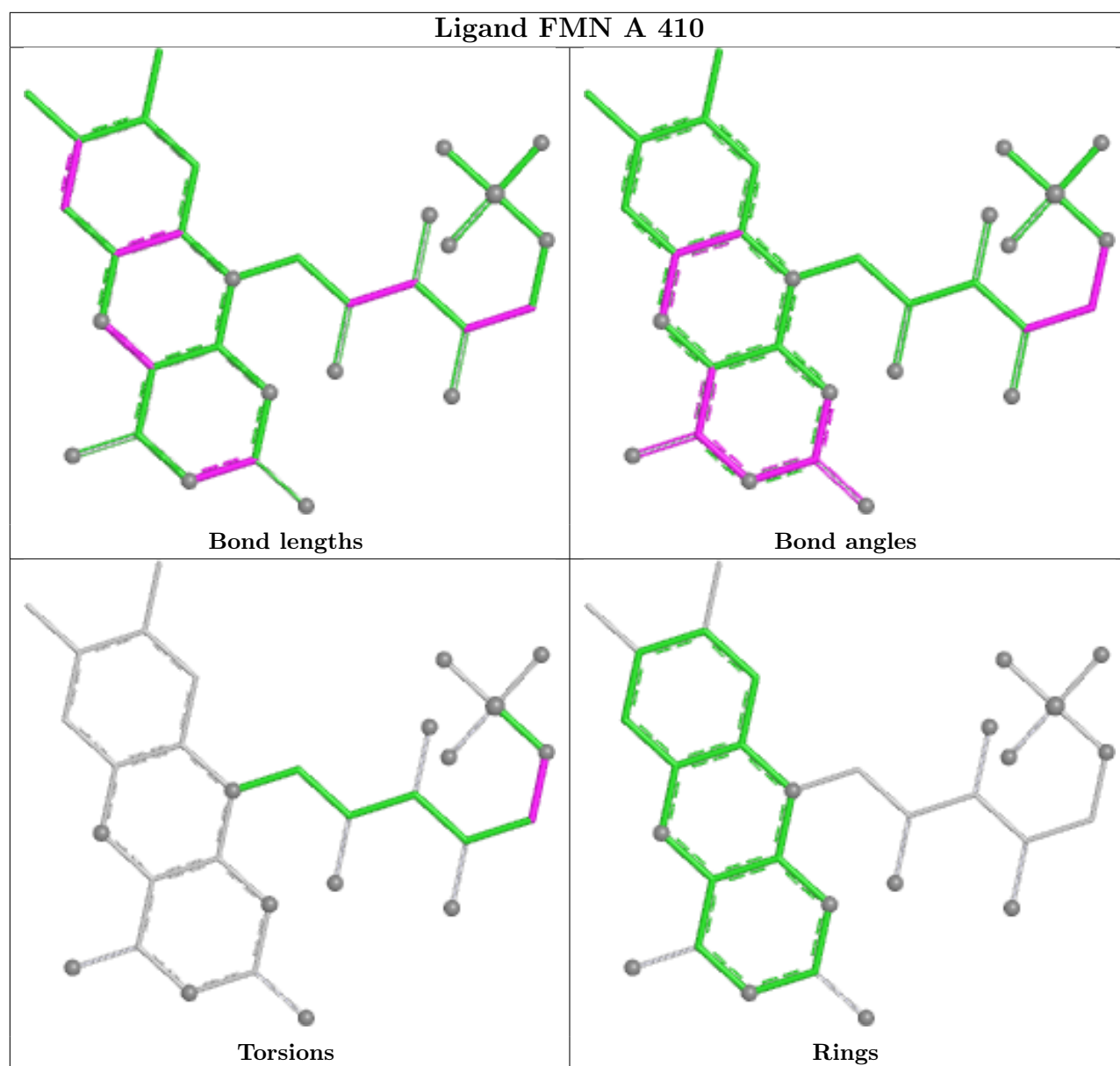
There are no ring outliers.

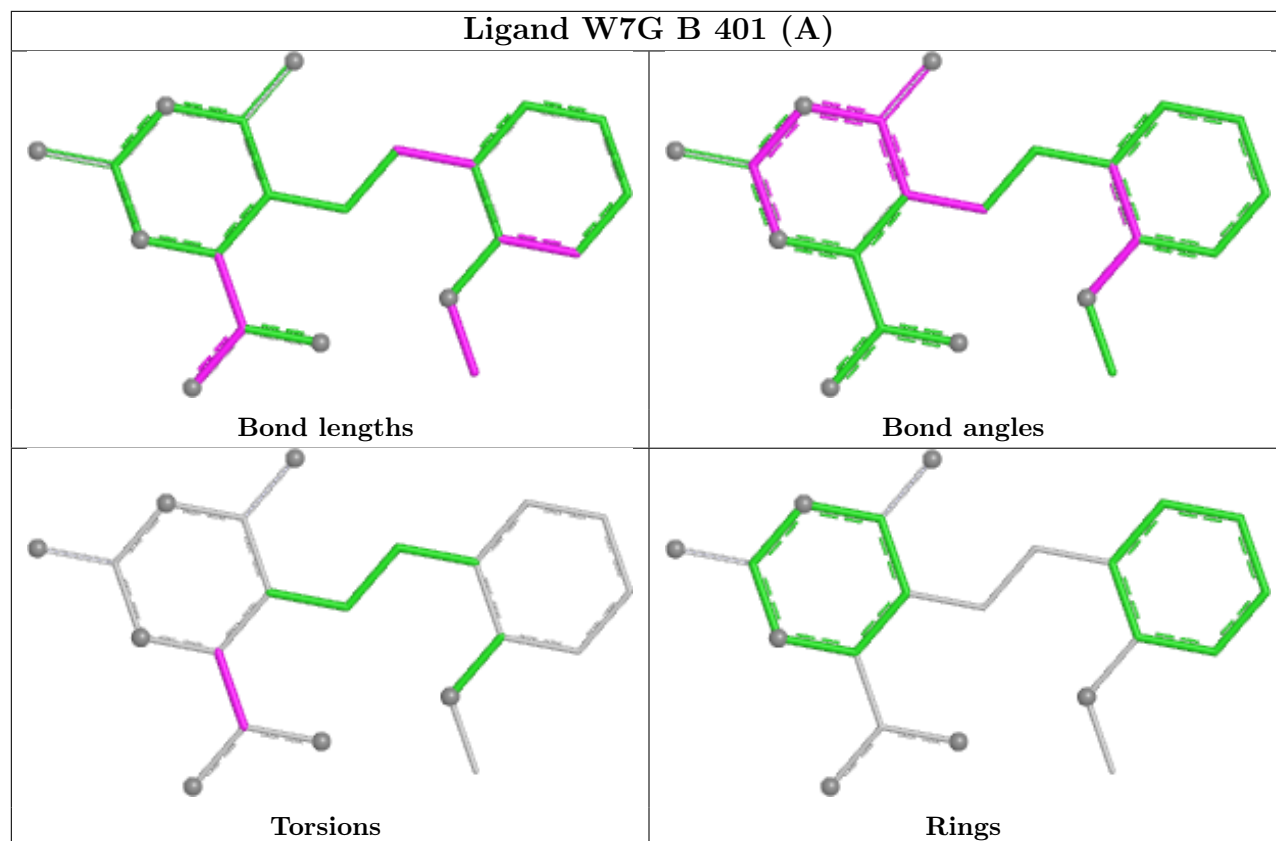
6 monomers are involved in 22 short contacts:

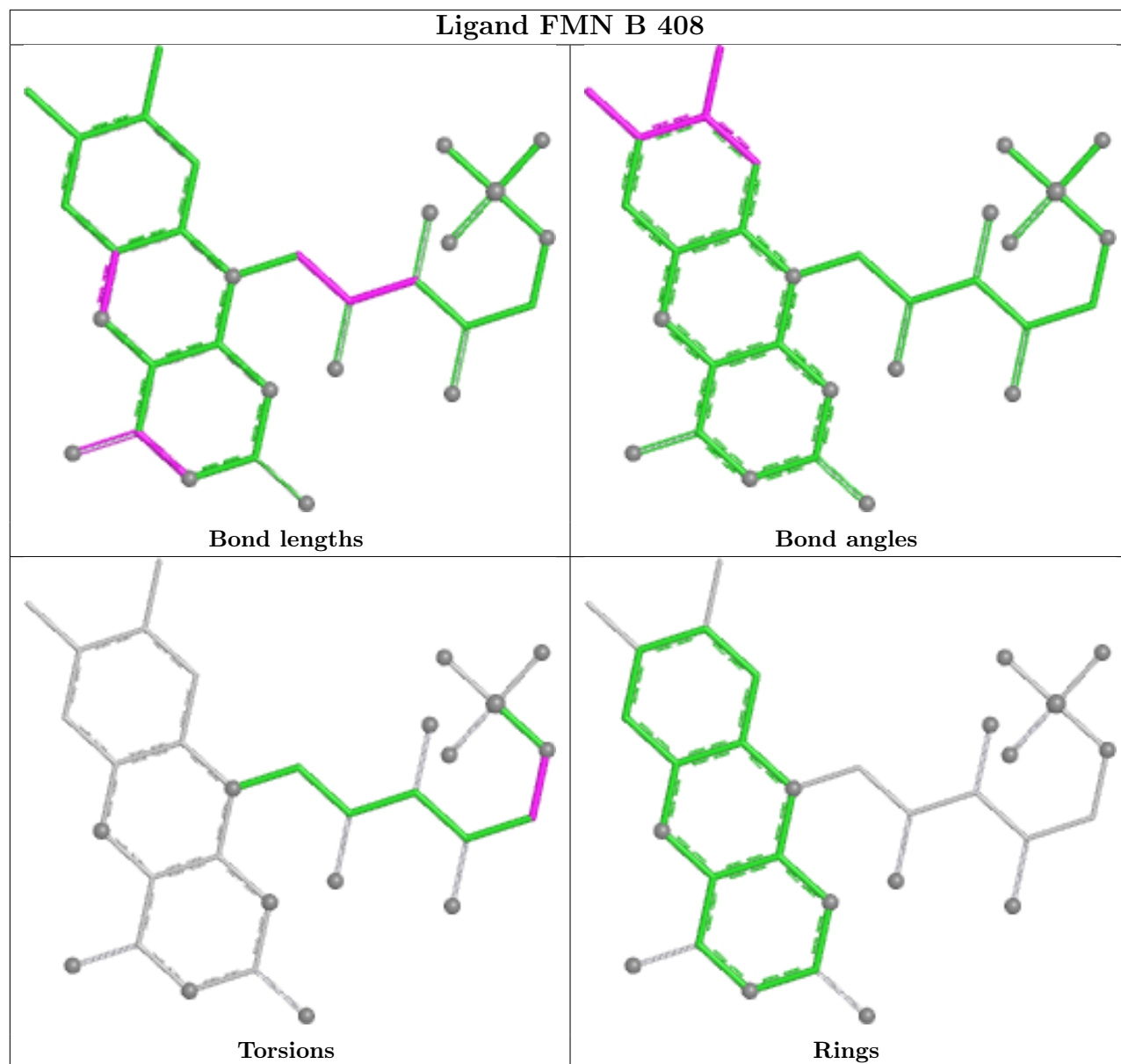
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	409	GOL	3	0
3	B	407	GOL	9	0
4	A	410	FMN	1	0
2	B	401[B]	W7G	7	0
3	B	402	GOL	1	0
3	A	403	GOL	1	0

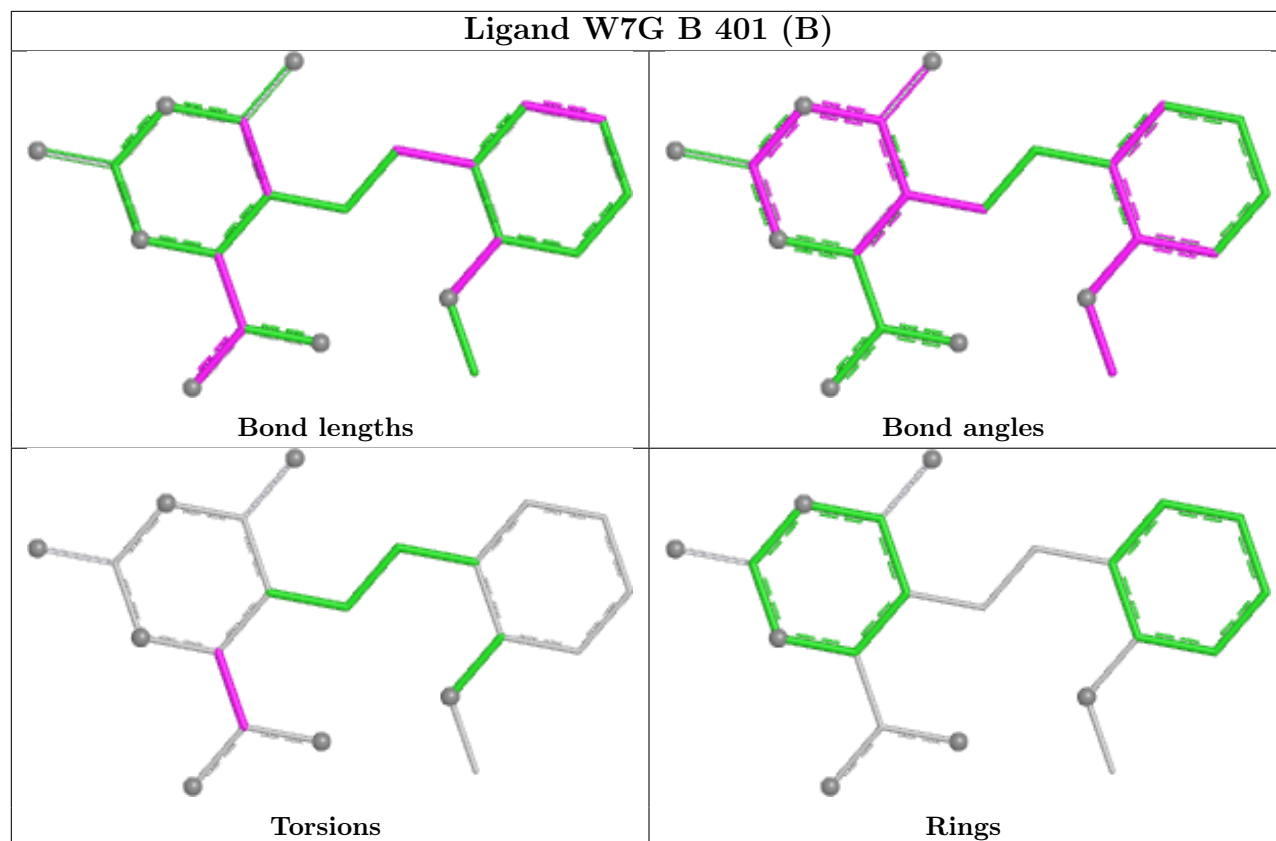
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 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.











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%)	-0.45	2 (0%) 85 89	6, 10, 20, 41	5 (1%)
1	B	313/313 (100%)	-0.24	9 (2%) 53 62	6, 11, 25, 46	3 (0%)
All	All	626/626 (100%)	-0.34	11 (1%) 67 76	6, 11, 24, 46	8 (1%)

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	131	PRO	5.6
1	B	135	GLY	3.2
1	B	130[A]	CYS	2.7
1	A	130	CYS	2.5
1	A	312	GLU	2.4
1	B	133	VAL	2.4
1	B	132	ASN	2.3
1	B	134	PRO	2.3
1	B	0	MET	2.2
1	B	5	ASN	2.1
1	B	1	CYS	2.1

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 ⓘ

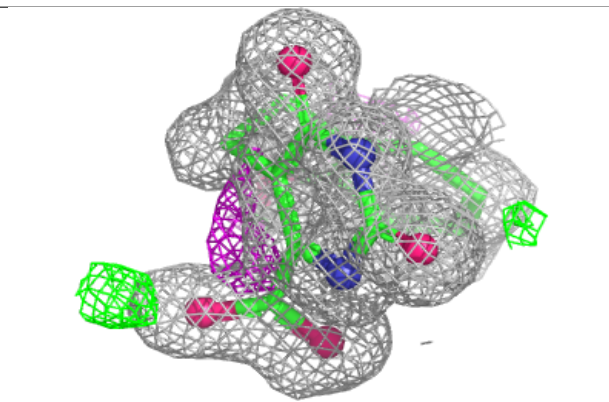
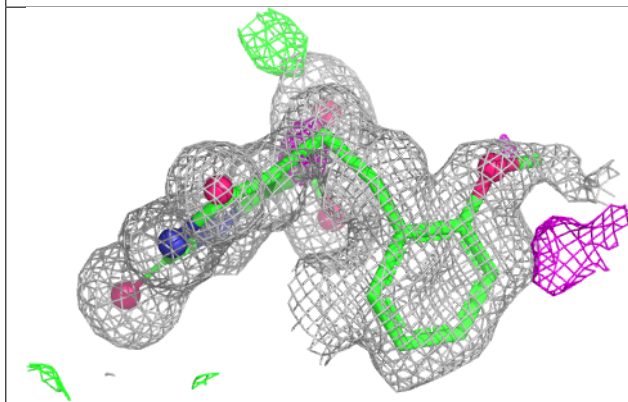
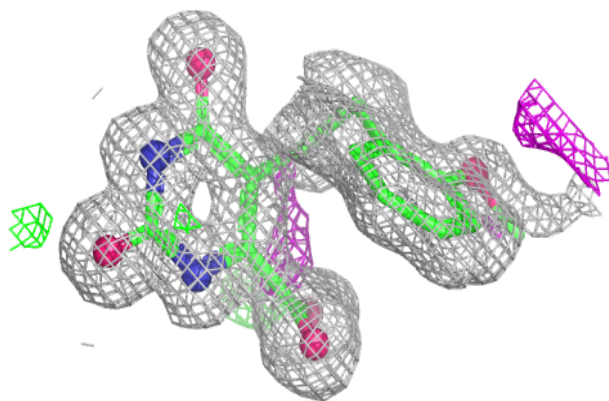
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists 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	404	6/6	0.78	0.14	33,39,42,44	0
3	GOL	A	402	6/6	0.80	0.14	29,37,39,39	0
3	GOL	A	406	6/6	0.81	0.16	55,55,59,62	0
3	GOL	B	406	6/6	0.81	0.12	31,35,36,39	0
3	GOL	B	402	6/6	0.87	0.13	28,44,46,50	0
3	GOL	B	403	6/6	0.87	0.12	27,32,37,42	0
3	GOL	B	407	6/6	0.87	0.12	25,35,38,41	0
3	GOL	A	409	6/6	0.88	0.11	36,40,43,44	0
3	GOL	A	405	6/6	0.88	0.10	23,26,28,31	0
3	GOL	A	403	6/6	0.90	0.11	23,28,32,39	0
3	GOL	A	404	6/6	0.90	0.12	27,29,32,32	0
3	GOL	B	405	6/6	0.95	0.06	16,17,19,20	0
2	W7G	B	401[B]	21/21	0.95	0.06	9,10,16,20	21
2	W7G	B	401[A]	21/21	0.95	0.06	8,10,12,13	21
3	GOL	A	407[B]	6/6	0.96	0.05	12,14,15,16	6
3	GOL	A	407[A]	6/6	0.96	0.05	12,15,16,17	6
3	GOL	A	408	6/6	0.97	0.05	15,17,19,21	0
2	W7G	A	401	21/21	0.97	0.04	8,9,11,12	0
4	FMN	A	410	31/31	0.98	0.04	6,7,9,14	0
4	FMN	B	408	31/31	0.99	0.04	6,7,9,12	0
5	NCO	A	411	7/7	0.99	0.07	10,10,12,12	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.

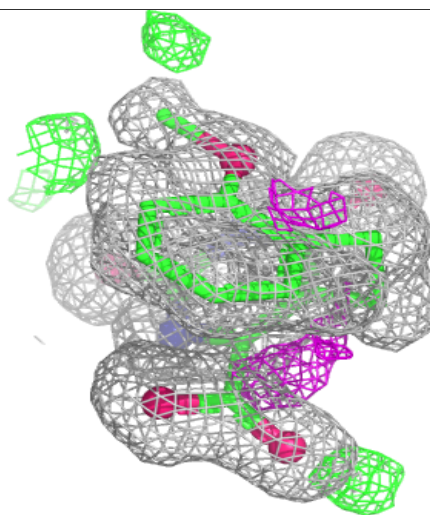
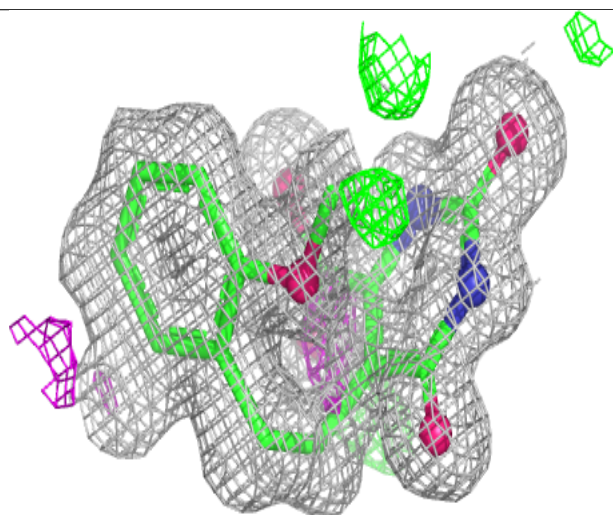
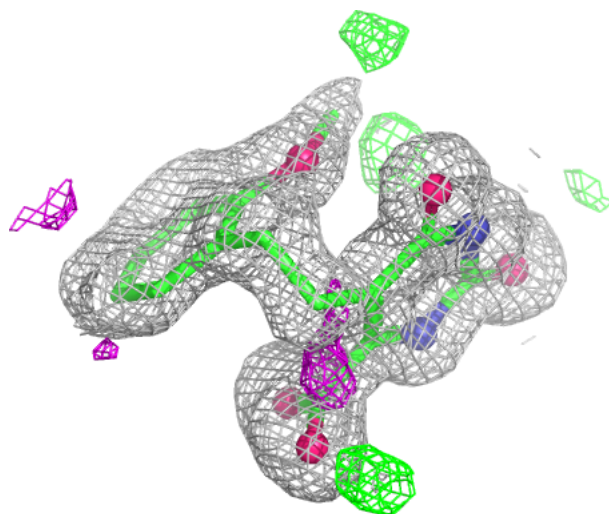
Electron density around W7G B 401 (B):

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



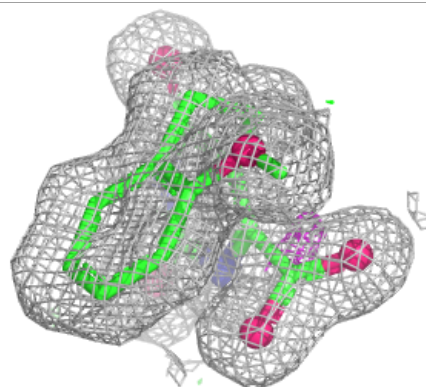
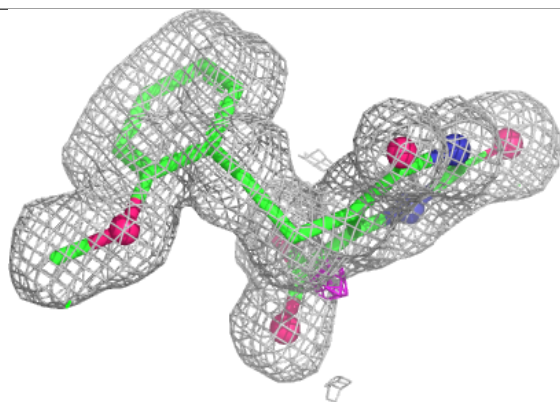
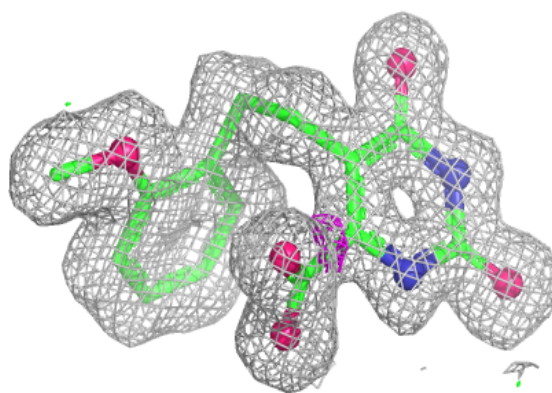
Electron density around W7G B 401 (A):

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



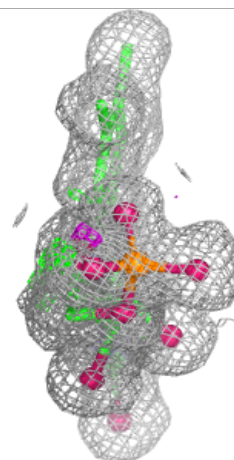
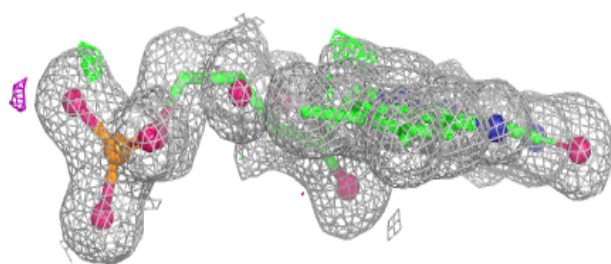
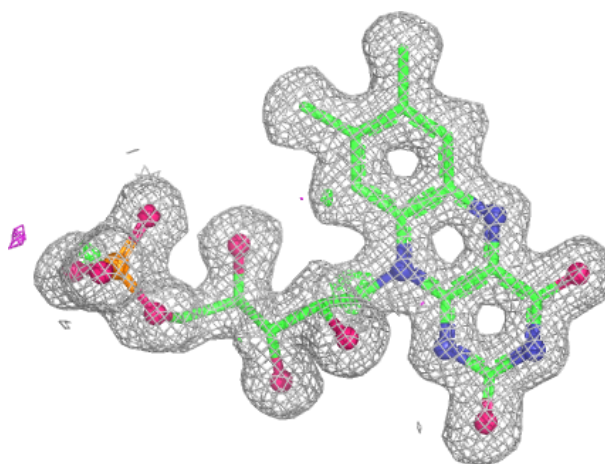
Electron density around W7G A 401:

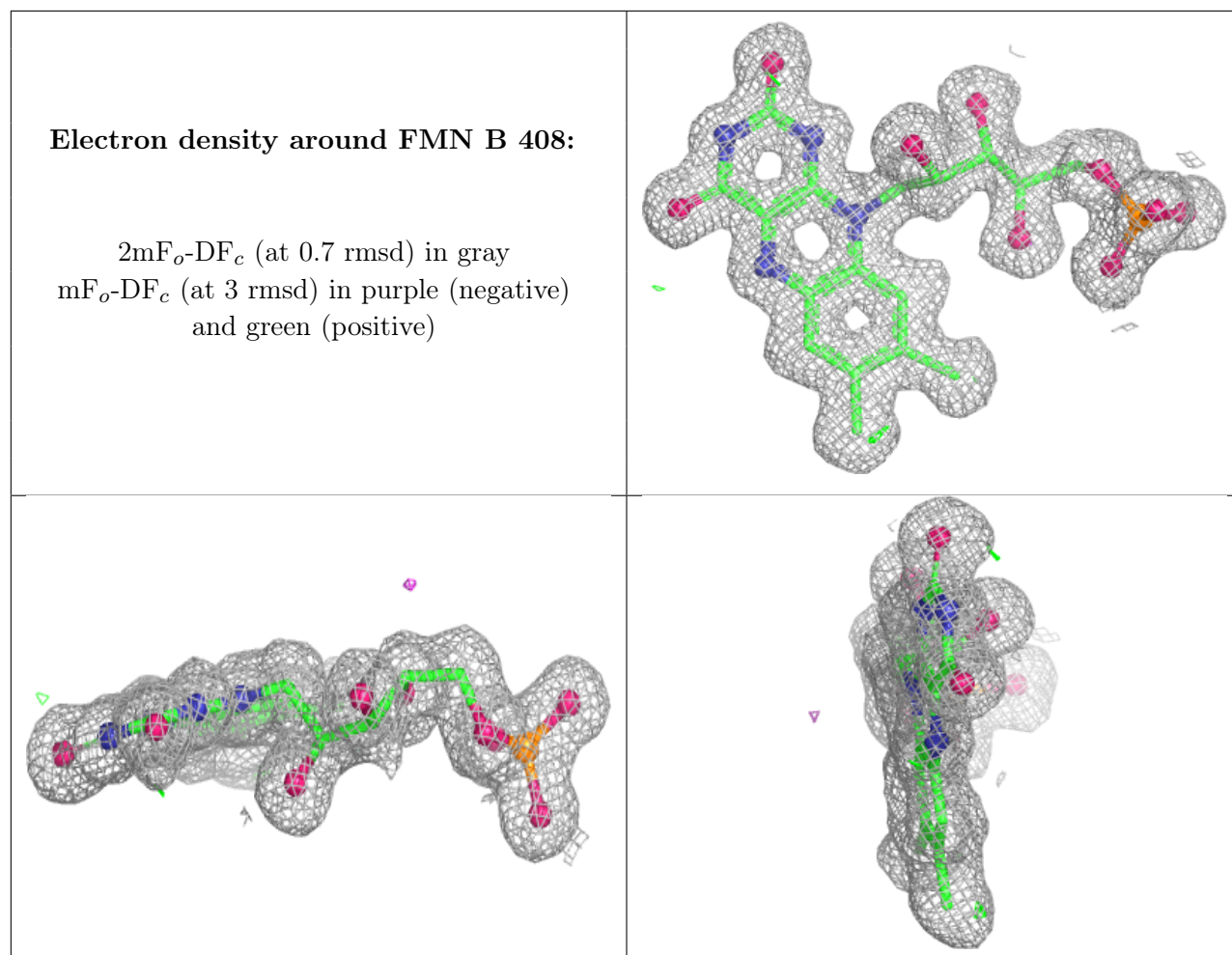
$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around FMN 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)





6.5 Other polymers ⓘ

There are no such residues in this entry.