



wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 18, 2026 – 03:46 PM UTC

PDB ID : 3W87 / pdb_00003w87
Title : Structure of Trypanosoma cruzi dihydroorotate dehydrogenase in complex with SH-1-103
Authors : Inaoka, D.K.; Hashimoto, S.; Rocha, J.R.; Iida, M.; Tabuchi, T.; Lee, N.; Matsuoka, S.; Kuranaga, T.; Shiba, T.; Balogun, E.O.; Sakamoto, K.; Suzuki, S.; Montanari, C.A.; Nara, T.; Aoki, T.; Inoue, M.; Honma, T.; Tanaka, A.; Harada, S.; Kita, K.
Deposited on : 2013-03-12
Resolution : 1.43 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

<https://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) 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	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)

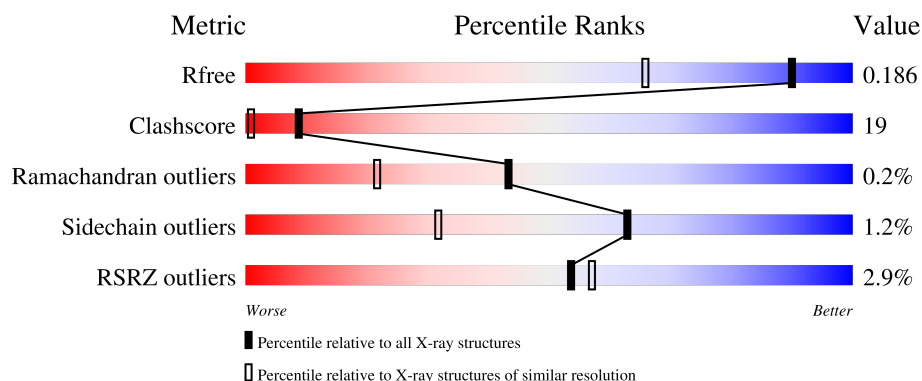
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.43 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	3234 (1.46-1.42)
Clashscore	190562	3289 (1.46-1.42)
Ramachandran outliers	187476	3248 (1.46-1.42)
Sidechain outliers	187428	3248 (1.46-1.42)
RSRZ outliers	180081	3234 (1.46-1.42)

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	314	4% 72% 25% ..
1	B	314	% 82% 16% .

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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
4	CAC	A	415	-	X	-	-
4	CAC	A	416	-	X	-	-
4	CAC	B	414	-	X	-	-
6	EDO	A	423	-	-	X	-
6	EDO	A	424	-	-	X	-
6	EDO	A	428	-	-	X	-
6	EDO	A	431	-	-	X	-
6	EDO	B	417	-	-	X	-
6	EDO	B	419	-	-	X	-
6	EDO	B	420	-	-	X	-
6	EDO	B	425	-	X	X	-
7	PEG	A	432	-	-	X	-
7	PEG	A	433	-	X	X	-
7	PEG	B	427	-	-	X	-

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 6373 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.

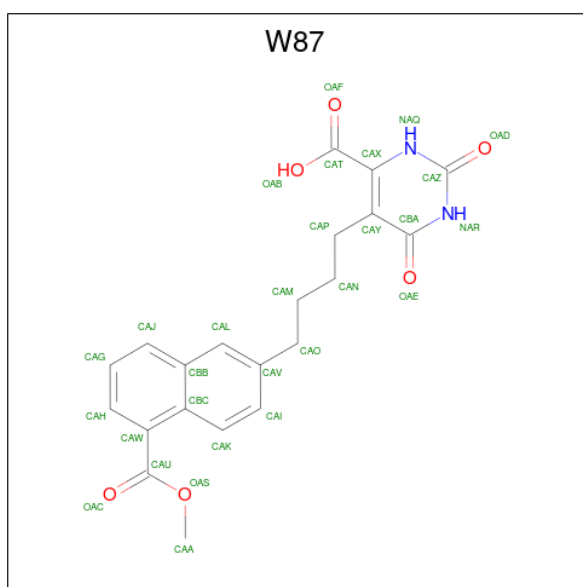
- Molecule 1 is a protein called Dihydroorotate dehydrogenase (fumarate).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	314	Total	C	N	O	S	0	18	0
			2540	1618	425	478	19			
1	B	314	Total	C	N	O	S	0	15	0
			2522	1603	423	477	19			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	SER	-	expression tag	UNP Q4D3W2
B	-1	SER	-	expression tag	UNP Q4D3W2

- Molecule 2 is 5-{4-[5-(methoxycarbonyl)naphthalen-2-yl]butyl}-2,6-dioxo-1,2,3,6-tetrahydro pyrimidine-4-carboxylic acid (CCD ID: W87) (formula: C₂₁H₂₀N₂O₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			29	21	2	6		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	N	O	0	1
			58	42	4	12		

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



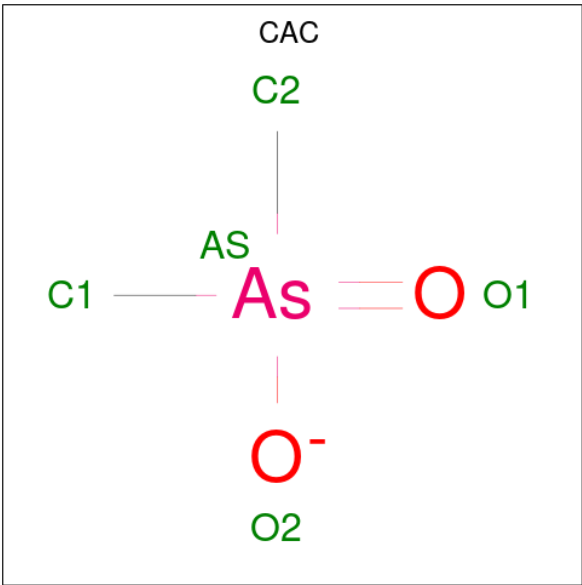
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	1
			12	6	6		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	1
			12	6	6		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total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

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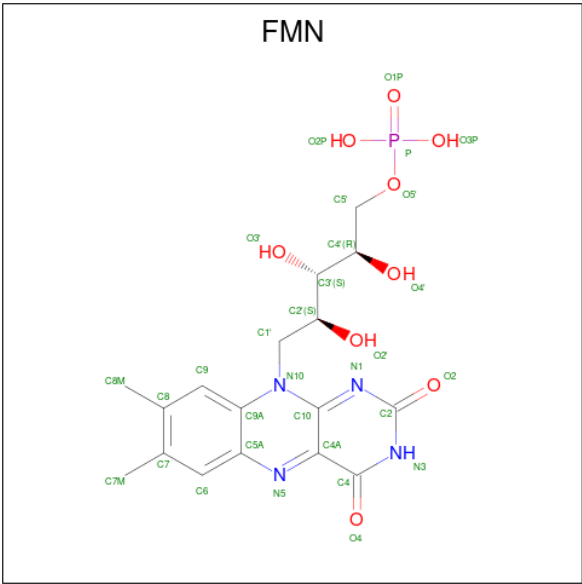
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	1
			12	6	6		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total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

- Molecule 4 is CACODYLATE ION (CCD ID: CAC) (formula: $C_2H_6AsO_2$).



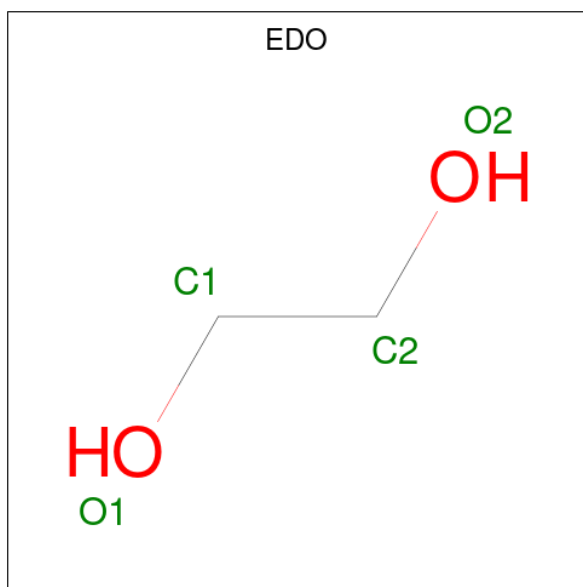
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	As	C	O	0	0
			5	1	2	2		
4	A	1	Total	As	C	O	0	0
			5	1	2	2		
4	B	1	Total	As	C	O	0	0
			5	1	2	2		
4	B	1	Total	As	C	O	0	0
			5	1	2	2		

- Molecule 5 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: C₁₇H₂₁N₄O₉P).



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

- Molecule 6 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



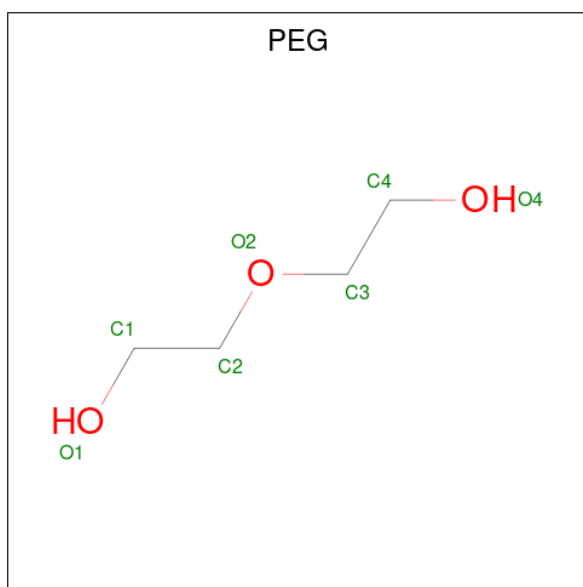
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		

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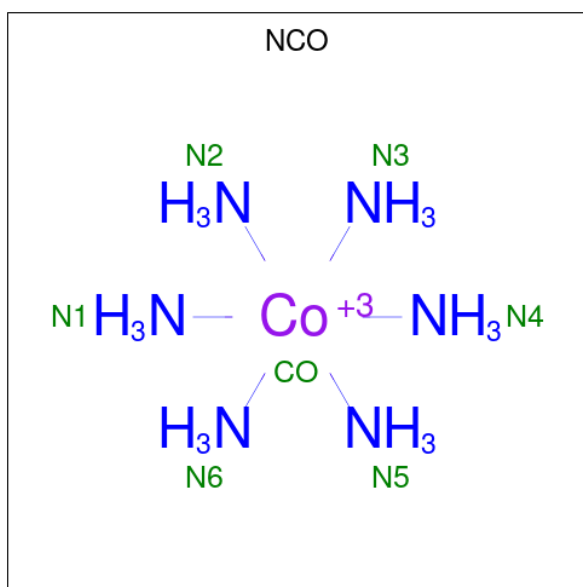
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		
6	B	1	Total	C	O	0	0
			4	2	2		
6	B	1	Total	C	O	0	0
			4	2	2		
6	B	1	Total	C	O	0	0
			4	2	2		
6	B	1	Total	C	O	0	0
			4	2	2		
6	B	1	Total	C	O	0	0
			4	2	2		
6	B	1	Total	C	O	0	0
			4	2	2		
6	B	1	Total	C	O	0	0
			4	2	2		
6	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 7 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			7	4	3		
7	A	1	Total	C	O	0	0
			7	4	3		
7	B	1	Total	C	O	0	0
			7	4	3		

- Molecule 8 is COBALT HEXAMMINE(III) (CCD ID: NCO) (formula: $\text{CoH}_{18}\text{N}_6$).



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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	Co	N	0	1
			14	2	12		

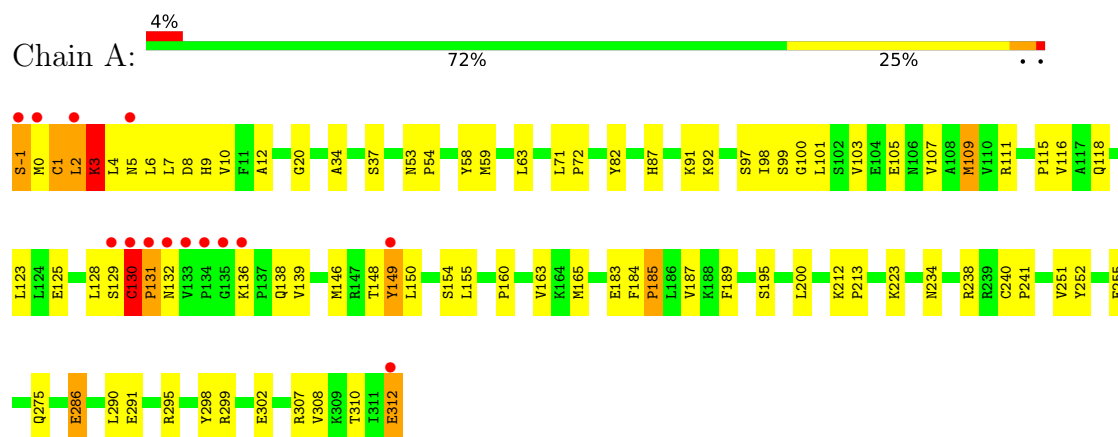
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	377	Total	O	0	9
			386	386		
9	B	444	Total	O	0	6
			450	450		

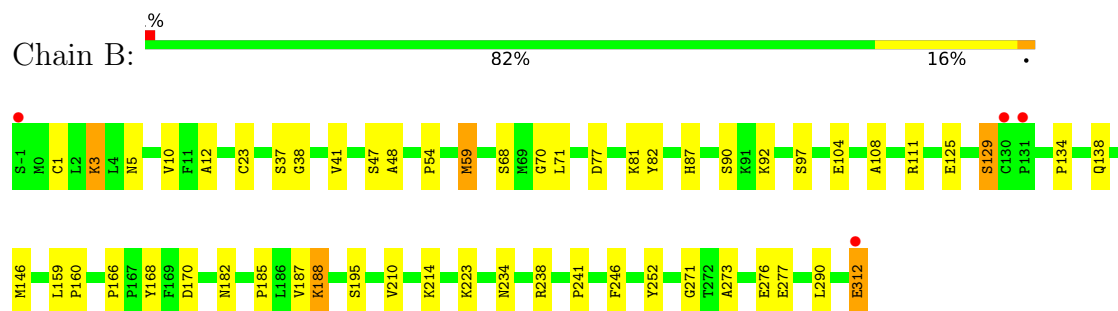
3 Residue-property plots [i](#)

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	67.93Å 71.48Å 129.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	36.98 – 1.43 36.98 – 1.43	Depositor EDS
% Data completeness (in resolution range)	97.3 (36.98-1.43) 97.3 (36.98-1.43)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.39 (at 1.43Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.153 , 0.187 0.152 , 0.186	Depositor DCC
R_{free} test set	5704 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å ²)	8.9	Xtriage
Anisotropy	0.008	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 43.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.005 for k,h,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	6373	wwPDB-VP
Average B, all atoms (Å ²)	13.0	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 26.97 % 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 2.3903e-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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: FMN, NCO, PEG, W87, CAC, EDO, GOL

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	1.69	32/2591 (1.2%)	1.43	11/3506 (0.3%)
1	B	1.64	16/2574 (0.6%)	1.35	10/3482 (0.3%)
All	All	1.67	48/5165 (0.9%)	1.39	21/6988 (0.3%)

The worst 5 of 48 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	146	MET	SD-CE	-14.73	1.42	1.79
1	B	3	LYS	CE-NZ	12.36	1.86	1.49
1	A	129	SER	CA-C	12.30	1.70	1.53
1	A	146	MET	SD-CE	-9.23	1.56	1.79
1	A	6	LEU	CA-CB	8.72	1.69	1.53

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	3	LYS	CD-CE-NZ	9.61	142.67	111.90
1	B	1	CYS	N-CA-CB	-8.77	96.15	110.71
1	B	146	MET	CG-SD-CE	-7.01	85.48	100.90
1	A	3	LYS	CA-CB-CG	6.99	128.08	114.10
1	A	148	THR	N-CA-C	6.97	119.47	111.11

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	2540	0	2524	119	0
1	B	2522	0	2501	57	0
2	A	29	0	19	1	0
2	B	58	0	38	3	0
3	A	90	0	119	12	0
3	B	78	0	102	10	0
4	A	10	0	0	2	0
4	B	10	0	0	0	0
5	A	31	0	19	1	0
5	B	31	0	19	0	0
6	A	56	0	84	33	0
6	B	40	0	59	34	0
7	A	14	0	19	21	0
7	B	7	0	10	8	0
8	A	21	0	0	4	0
9	A	386	0	0	23	0
9	B	450	0	0	23	0
All	All	6373	0	5513	208	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 19.

The worst 5 of 208 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:3:LYS:CE	1:B:3:LYS:NZ	1.86	1.38
1:A:2:LEU:HD12	1:A:286:GLU:HG3	1.18	1.09
1:A:4[B]:LEU:C	1:A:4[B]:LEU:HD12	1.73	1.09
1:A:128:LEU:CD1	1:A:163[B]:VAL:HG21	1.85	1.06
1:A:1:CYS:HB2	7:A:433:PEG:H22	1.26	1.06

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	329/314 (105%)	318 (97%)	10 (3%)	1 (0%)	36	17
1	B	328/314 (104%)	316 (96%)	12 (4%)	0	100	100
All	All	657/628 (105%)	634 (96%)	22 (3%)	1 (0%)	43	22

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	0	MET

5.3.2 Protein sidechains ⓘ

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	277/259 (107%)	270 (98%)	7 (2%)	42	10
1	B	275/259 (106%)	274 (100%)	1 (0%)	84	69
All	All	552/518 (107%)	544 (99%)	8 (1%)	63	26

5 of 8 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	312	GLU
1	A	312[B]	GLU
1	A	130[B]	CYS
1	A	130[A]	CYS
1	A	312[A]	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	132	ASN

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Mol	Chain	Res	Type
1	B	138	GLN
1	B	275	GLN
1	B	234	ASN
1	A	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](#)

67 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	W87	B	401[A]	-	31,31,31	1.93	8 (25%)	41,43,43	1.95	12 (29%)
2	W87	A	401	-	31,31,31	1.60	3 (9%)	41,43,43	2.19	17 (41%)
3	GOL	A	404	-	5,5,5	0.88	0	5,5,5	2.33	3 (60%)
3	GOL	B	405[B]	-	5,5,5	0.36	0	5,5,5	1.24	0
3	GOL	A	409	-	5,5,5	0.81	0	5,5,5	1.53	2 (40%)
3	GOL	B	410	-	5,5,5	0.25	0	5,5,5	0.83	0
6	EDO	A	429	-	3,3,3	0.38	0	2,2,2	0.81	0
7	PEG	B	427	-	6,6,6	1.25	1 (16%)	5,5,5	1.76	1 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	NCO	A	435[A]	-	6,6,6	2.68	3 (50%)	-		
3	GOL	A	410	-	5,5,5	0.40	0	5,5,5	0.67	0
3	GOL	A	411	-	5,5,5	0.59	0	5,5,5	1.36	1 (20%)
3	GOL	B	404	-	5,5,5	1.30	1 (20%)	5,5,5	1.04	0
5	FMN	A	417	-	33,33,33	1.15	2 (6%)	48,50,50	1.15	4 (8%)
3	GOL	B	408	-	5,5,5	0.53	0	5,5,5	0.70	0
3	GOL	A	406[B]	-	5,5,5	0.23	0	5,5,5	0.71	0
3	GOL	A	408	-	5,5,5	0.48	0	5,5,5	0.74	0
3	GOL	B	407	-	5,5,5	0.46	0	5,5,5	0.88	0
4	CAC	A	416	-	2,4,4	3.21	1 (50%)	4,6,6	16.87	4 (100%)
5	FMN	B	416	-	33,33,33	1.38	6 (18%)	48,50,50	1.28	5 (10%)
6	EDO	A	427	-	3,3,3	0.81	0	2,2,2	0.15	0
3	GOL	A	413	-	5,5,5	0.76	0	5,5,5	0.80	0
6	EDO	A	430	-	3,3,3	0.87	0	2,2,2	0.60	0
6	EDO	B	418	-	3,3,3	0.29	0	2,2,2	1.05	0
3	GOL	A	402[A]	-	5,5,5	1.05	0	5,5,5	0.42	0
6	EDO	A	426	-	3,3,3	0.50	0	2,2,2	0.25	0
6	EDO	B	426	-	3,3,3	0.78	0	2,2,2	0.62	0
6	EDO	B	420	-	3,3,3	0.92	0	2,2,2	0.86	0
6	EDO	B	423	-	3,3,3	0.45	0	2,2,2	0.59	0
6	EDO	A	423	-	3,3,3	0.52	0	2,2,2	0.50	0
6	EDO	A	431	-	3,3,3	1.61	1 (33%)	2,2,2	1.52	0
6	EDO	A	428	-	3,3,3	0.47	0	2,2,2	0.59	0
4	CAC	A	415	-	2,4,4	4.34	1 (50%)	4,6,6	11.24	3 (75%)
3	GOL	B	406	-	5,5,5	0.99	0	5,5,5	1.48	1 (20%)
6	EDO	A	418	-	3,3,3	0.81	0	2,2,2	0.30	0
6	EDO	B	425	-	3,3,3	1.29	1 (33%)	2,2,2	1.98	1 (50%)
3	GOL	B	403	-	5,5,5	0.59	0	5,5,5	0.92	0
3	GOL	B	405[A]	-	5,5,5	0.73	0	5,5,5	0.85	0
3	GOL	A	412	-	5,5,5	0.58	0	5,5,5	0.74	0
6	EDO	B	424	-	3,3,3	0.56	0	2,2,2	0.33	0
2	W87	B	401[B]	-	31,31,31	1.80	7 (22%)	41,43,43	1.80	9 (21%)
3	GOL	B	413	-	5,5,5	0.41	0	5,5,5	1.18	0
3	GOL	B	411	-	5,5,5	0.54	0	5,5,5	1.19	1 (20%)
6	EDO	A	424	-	3,3,3	0.58	0	2,2,2	0.29	0
6	EDO	B	421	-	3,3,3	0.82	0	2,2,2	0.50	0
3	GOL	A	406[A]	-	5,5,5	0.51	0	5,5,5	0.49	0
6	EDO	A	421	-	3,3,3	0.36	0	2,2,2	1.96	1 (50%)
6	EDO	A	425	-	3,3,3	0.66	0	2,2,2	0.36	0
6	EDO	B	419	-	3,3,3	0.61	0	2,2,2	0.46	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	NCO	A	435[B]	-	6,6,6	2.75	4 (66%)	-		
7	PEG	A	432	-	6,6,6	1.06	1 (16%)	5,5,5	1.09	0
3	GOL	A	407	-	5,5,5	0.40	0	5,5,5	0.44	0
6	EDO	B	417	-	3,3,3	1.23	0	2,2,2	1.24	0
6	EDO	A	419	-	3,3,3	0.51	0	2,2,2	0.46	0
6	EDO	B	422	-	3,3,3	0.66	0	2,2,2	0.23	0
6	EDO	A	422	-	3,3,3	0.36	0	2,2,2	1.10	0
8	NCO	A	434	-	6,6,6	5.76	6 (100%)	-		
3	GOL	A	402[B]	-	5,5,5	1.31	0	5,5,5	1.07	0
3	GOL	A	405	-	5,5,5	0.98	0	5,5,5	1.32	1 (20%)
7	PEG	A	433	-	6,6,6	1.03	1 (16%)	5,5,5	2.22	1 (20%)
3	GOL	A	414	-	5,5,5	0.41	0	5,5,5	0.36	0
4	CAC	B	415	-	2,4,4	2.82	2 (100%)	4,6,6	1.46	0
3	GOL	B	402	-	5,5,5	0.68	0	5,5,5	0.71	0
3	GOL	B	409	-	5,5,5	0.95	0	5,5,5	0.91	0
3	GOL	A	403	-	5,5,5	0.66	0	5,5,5	1.18	1 (20%)
6	EDO	A	420	-	3,3,3	0.60	0	2,2,2	0.76	0
3	GOL	B	412	-	5,5,5	0.39	0	5,5,5	0.84	0
4	CAC	B	414	-	2,4,4	2.38	1 (50%)	4,6,6	5.20	4 (100%)

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	W87	B	401[A]	-	-	9/17/17/17	0/3/3/3
2	W87	A	401	-	-	6/17/17/17	0/3/3/3
3	GOL	A	404	-	-	2/4/4/4	-
3	GOL	B	405[B]	-	-	3/4/4/4	-
3	GOL	A	409	-	-	0/4/4/4	-
3	GOL	B	410	-	-	0/4/4/4	-
6	EDO	A	429	-	-	1/1/1/1	-
7	PEG	B	427	-	-	3/4/4/4	-
3	GOL	A	410	-	-	4/4/4/4	-
3	GOL	A	411	-	-	4/4/4/4	-
3	GOL	B	404	-	-	0/4/4/4	-
5	FMN	A	417	-	-	1/18/18/18	0/3/3/3
3	GOL	B	408	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	A	406[B]	-	-	1/4/4/4	-
3	GOL	A	408	-	-	3/4/4/4	-
3	GOL	B	407	-	-	3/4/4/4	-
5	FMN	B	416	-	-	2/18/18/18	0/3/3/3
6	EDO	A	430	-	-	1/1/1/1	-
6	EDO	A	427	-	-	1/1/1/1	-
3	GOL	A	413	-	-	4/4/4/4	-
6	EDO	B	418	-	-	0/1/1/1	-
6	EDO	B	426	-	-	0/1/1/1	-
3	GOL	A	402[A]	-	-	0/4/4/4	-
6	EDO	A	426	-	-	1/1/1/1	-
6	EDO	B	420	-	-	1/1/1/1	-
6	EDO	B	423	-	-	1/1/1/1	-
6	EDO	A	423	-	-	1/1/1/1	-
6	EDO	A	431	-	-	1/1/1/1	-
6	EDO	A	428	-	-	0/1/1/1	-
3	GOL	B	406	-	-	0/4/4/4	-
6	EDO	A	418	-	-	1/1/1/1	-
6	EDO	B	425	-	-	1/1/1/1	-
3	GOL	B	403	-	-	4/4/4/4	-
3	GOL	B	405[A]	-	-	1/4/4/4	-
3	GOL	A	412	-	-	0/4/4/4	-
6	EDO	B	424	-	-	1/1/1/1	-
2	W87	B	401[B]	-	-	13/17/17/17	0/3/3/3
3	GOL	B	413	-	-	4/4/4/4	-
3	GOL	B	411	-	-	2/4/4/4	-
6	EDO	A	424	-	-	0/1/1/1	-
6	EDO	B	421	-	-	1/1/1/1	-
3	GOL	A	406[A]	-	-	4/4/4/4	-
6	EDO	A	421	-	-	1/1/1/1	-
6	EDO	A	425	-	-	0/1/1/1	-
6	EDO	B	419	-	-	0/1/1/1	-
7	PEG	A	432	-	-	2/4/4/4	-
3	GOL	A	407	-	-	1/4/4/4	-
6	EDO	B	417	-	-	0/1/1/1	-
6	EDO	A	419	-	-	0/1/1/1	-
6	EDO	B	422	-	-	1/1/1/1	-
6	EDO	A	422	-	-	1/1/1/1	-
3	GOL	A	402[B]	-	-	0/4/4/4	-
3	GOL	A	405	-	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	PEG	A	433	-	-	4/4/4/4	-
3	GOL	A	414	-	-	3/4/4/4	-
3	GOL	B	402	-	-	0/4/4/4	-
3	GOL	B	409	-	-	4/4/4/4	-
3	GOL	A	403	-	-	0/4/4/4	-
6	EDO	A	420	-	-	0/1/1/1	-
3	GOL	B	412	-	-	0/4/4/4	-

The worst 5 of 50 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	434	NCO	CO-N5	8.61	2.24	1.96
8	A	434	NCO	CO-N3	6.83	2.18	1.96
4	A	415	CAC	AS-C1	6.06	2.04	1.90
2	B	401[B]	W87	OAS-CAU	5.95	1.46	1.33
2	B	401[A]	W87	OAS-CAU	5.90	1.46	1.33

The worst 5 of 72 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	416	CAC	O1-AS-C2	-27.88	76.83	111.50
4	A	416	CAC	O2-AS-C2	17.22	147.56	105.84
4	A	415	CAC	O1-AS-C2	16.10	131.52	111.50
4	A	415	CAC	O1-AS-C1	-15.54	92.17	111.50
4	A	416	CAC	O1-AS-C1	-6.50	103.41	111.50

There are no chirality outliers.

5 of 104 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	W87	OAB-CAT-CAX-NAQ
2	B	401[A]	W87	OAB-CAT-CAX-NAQ
2	B	401[B]	W87	OAB-CAT-CAX-NAQ
3	A	404	GOL	C1-C2-C3-O3
3	A	406[A]	GOL	O1-C1-C2-O2

There are no ring outliers.

44 monomers are involved in 125 short contacts:

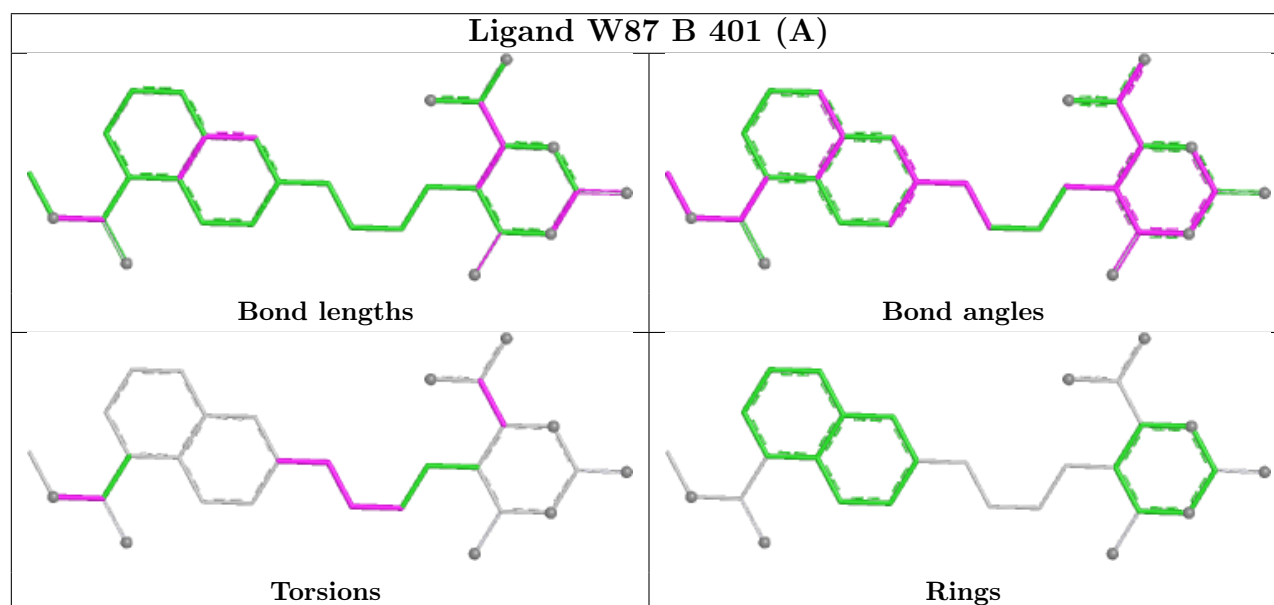
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	401[A]	W87	1	0
2	A	401	W87	1	0
3	A	409	GOL	2	0
3	B	410	GOL	2	0
7	B	427	PEG	8	0
3	A	410	GOL	1	0
3	A	411	GOL	3	0
5	A	417	FMN	1	0
3	B	408	GOL	1	0
3	A	406[B]	GOL	1	0
4	A	416	CAC	1	0
6	A	427	EDO	2	0
3	A	413	GOL	1	0
6	A	430	EDO	1	0
6	B	418	EDO	1	0
3	A	402[A]	GOL	1	0
6	A	426	EDO	2	0
6	B	426	EDO	1	0
6	B	420	EDO	5	0
6	B	423	EDO	3	0
6	A	423	EDO	5	0
6	A	431	EDO	8	0
6	A	428	EDO	4	0
4	A	415	CAC	1	0
6	A	418	EDO	3	0
6	B	425	EDO	6	0
3	B	403	GOL	1	0
2	B	401[B]	W87	2	0
3	B	413	GOL	3	0
3	B	411	GOL	1	0
6	A	424	EDO	4	0
6	B	421	EDO	2	0
6	A	421	EDO	1	0
6	A	425	EDO	1	0
6	B	419	EDO	4	0
7	A	432	PEG	5	0
6	B	417	EDO	9	0
6	B	422	EDO	3	0
8	A	434	NCO	4	0
7	A	433	PEG	16	0
3	A	414	GOL	2	0
3	B	409	GOL	2	0
3	A	403	GOL	1	0

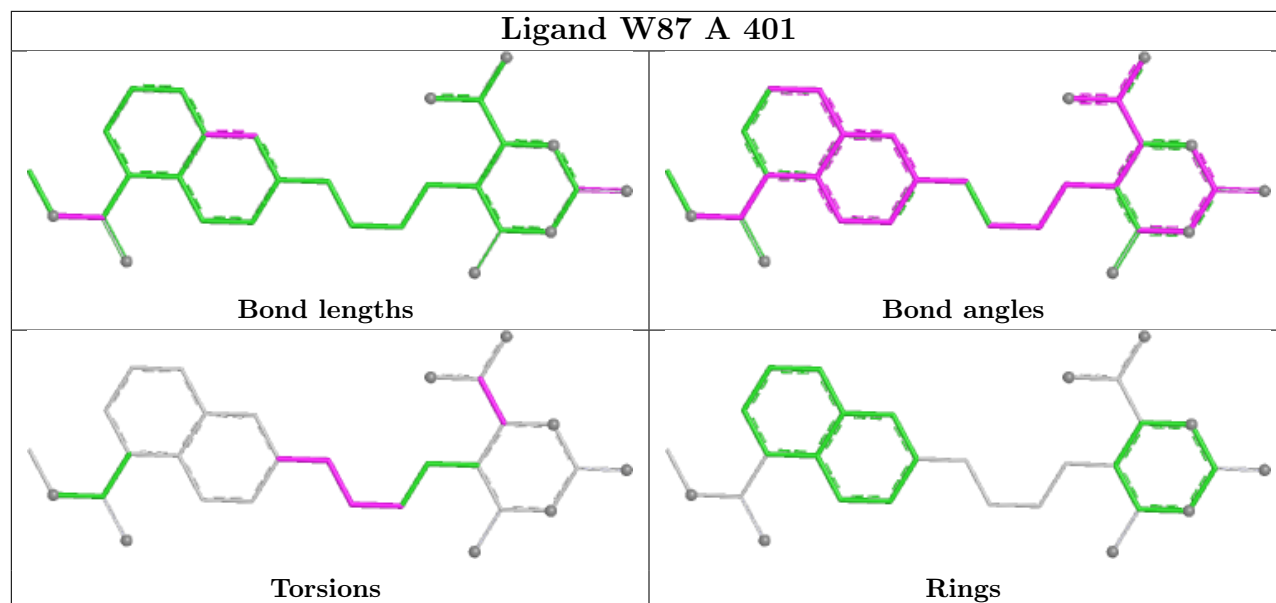
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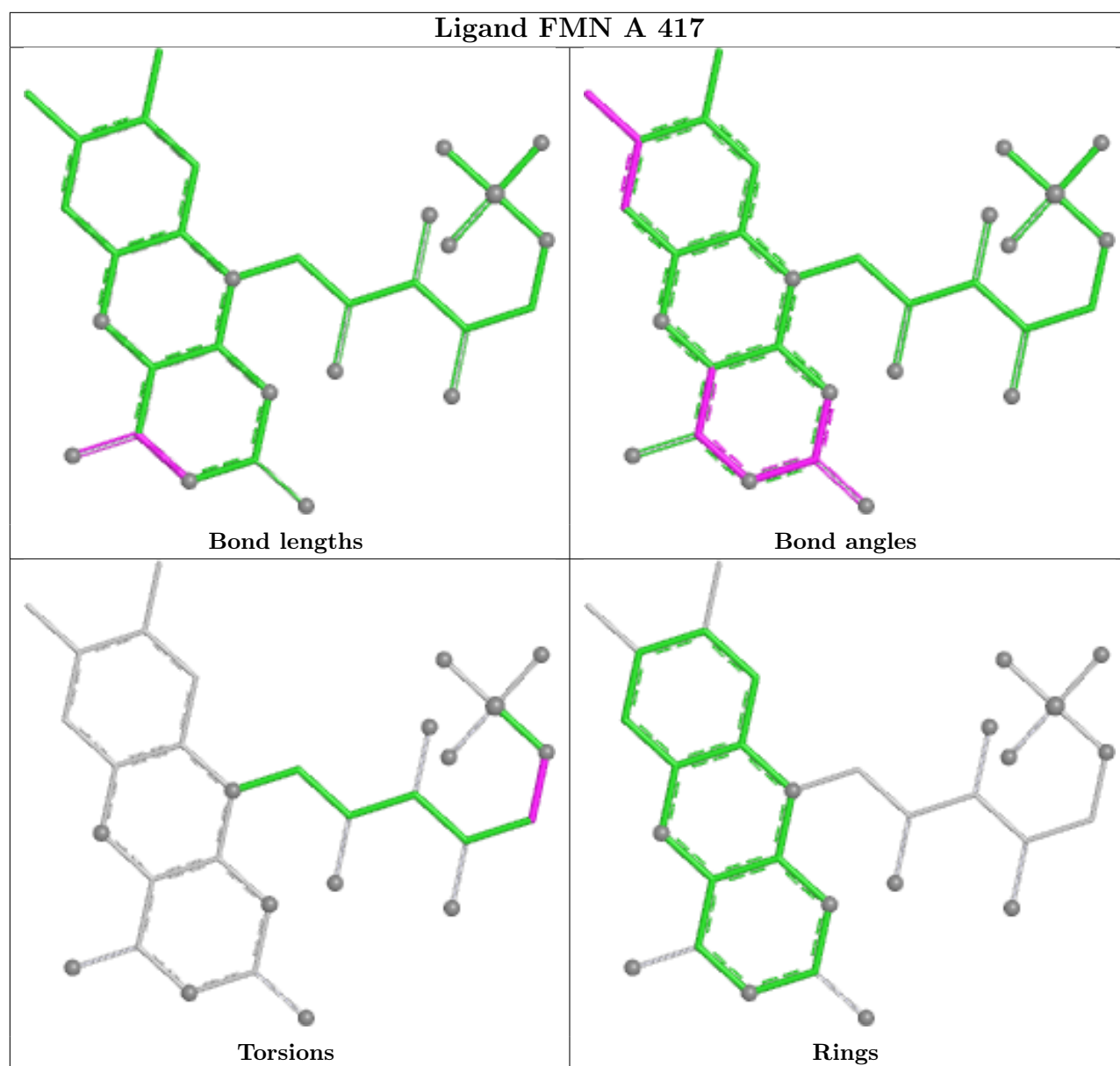
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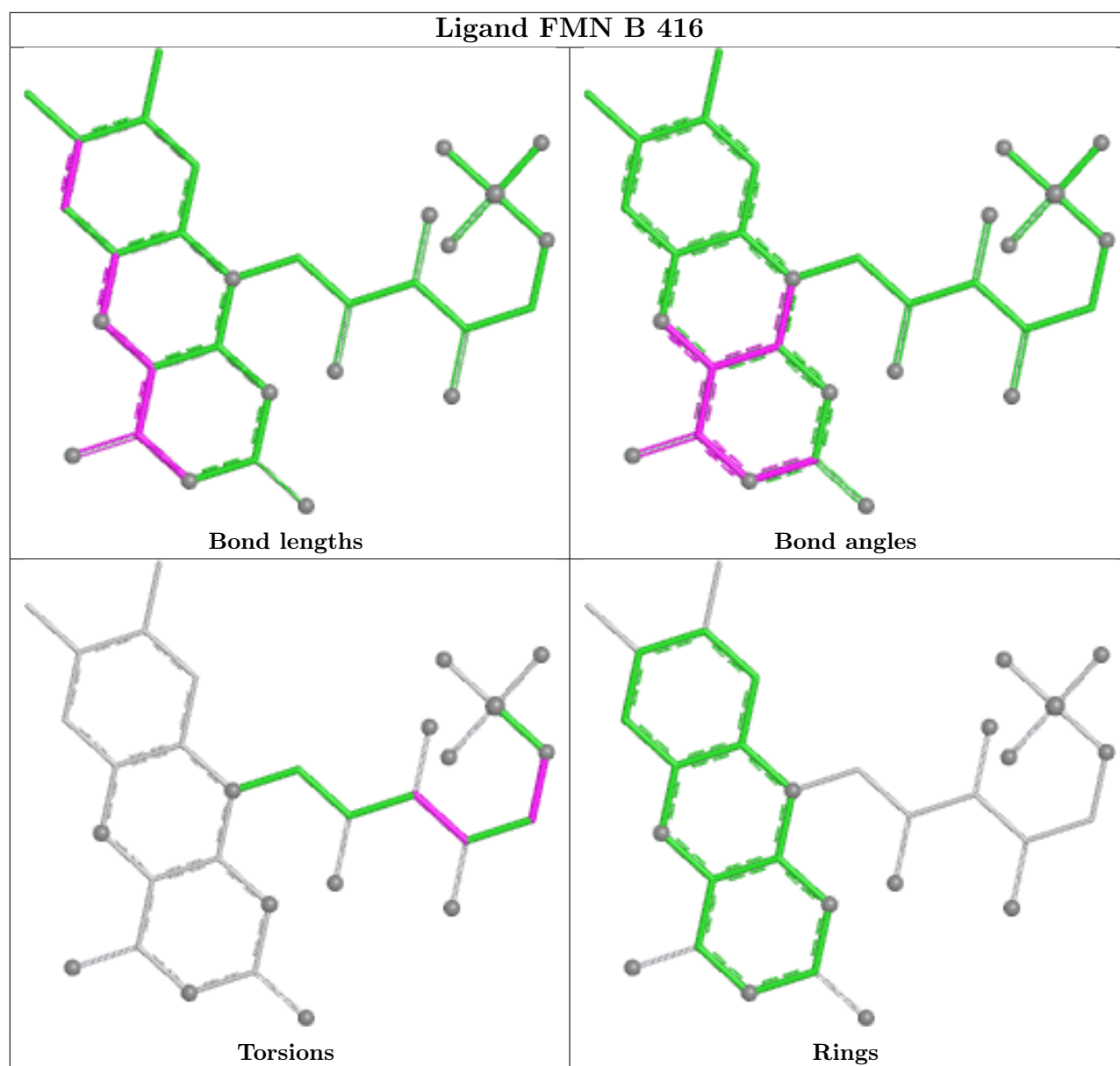
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	420	EDO	3	0

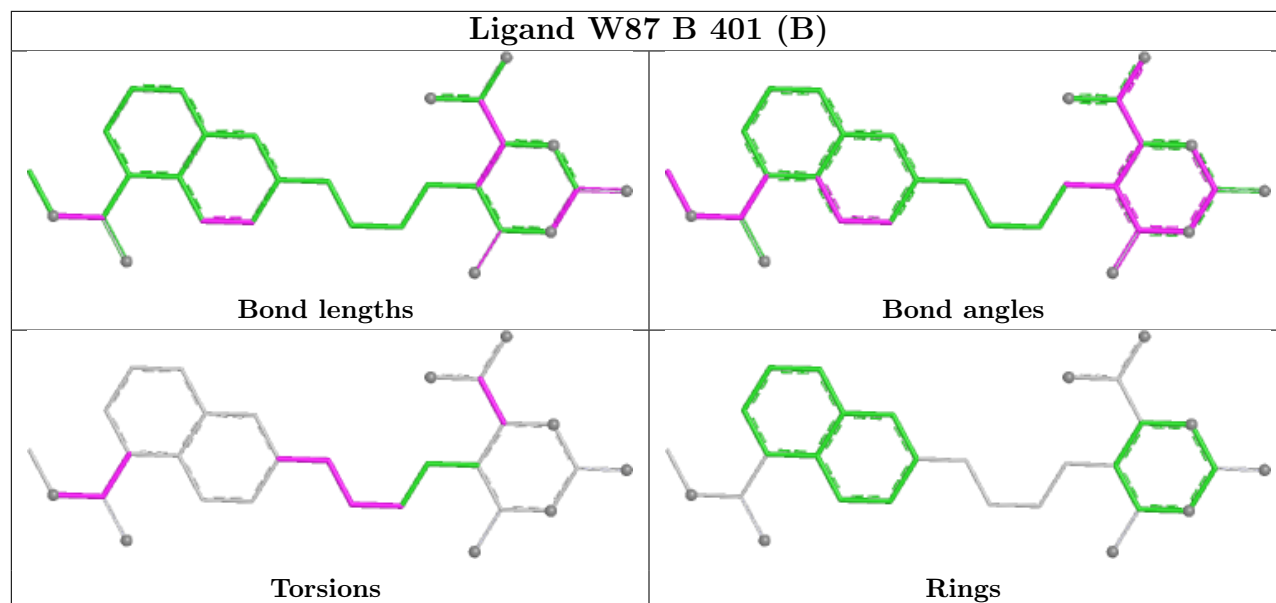
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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	314/314 (100%)	-0.29	14 (4%) 38 41	3, 8, 23, 41	18 (5%)
1	B	314/314 (100%)	-0.53	4 (1%) 75 79	3, 8, 19, 36	15 (4%)
All	All	628/628 (100%)	-0.41	18 (2%) 53 57	3, 8, 21, 41	33 (5%)

The worst 5 of 18 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	131	PRO	5.8
1	A	133	VAL	4.7
1	A	134	PRO	4.6
1	A	130[A]	CYS	4.2
1	A	-1	SER	3.9

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	GOL	A	410	6/6	0.44	0.21	50,56,58,62	0
4	CAC	B	415	5/5	0.52	0.26	169,169,169,169	0
6	EDO	A	429	4/4	0.65	0.22	51,52,52,53	0
6	EDO	A	427	4/4	0.68	0.19	39,48,48,52	0
3	GOL	A	407	6/6	0.70	0.18	38,51,54,55	0
6	EDO	A	419	4/4	0.71	0.16	53,53,54,55	0
6	EDO	B	422	4/4	0.71	0.19	41,42,43,44	0
6	EDO	B	424	4/4	0.71	0.17	47,47,50,51	0
3	GOL	B	412	6/6	0.73	0.16	49,50,50,51	0
6	EDO	A	426	4/4	0.76	0.15	53,54,54,55	0
3	GOL	A	414	6/6	0.77	0.15	33,48,49,52	0
3	GOL	A	406[A]	6/6	0.77	0.18	35,37,38,41	6
3	GOL	A	406[B]	6/6	0.77	0.18	16,26,27,28	6
3	GOL	B	413	6/6	0.78	0.14	27,46,48,51	0
3	GOL	B	409	6/6	0.78	0.14	29,35,36,43	0
6	EDO	B	421	4/4	0.79	0.14	33,34,40,41	0
6	EDO	A	425	4/4	0.79	0.14	33,35,37,39	0
3	GOL	B	403	6/6	0.79	0.15	20,34,36,37	0
6	EDO	B	418	4/4	0.80	0.16	35,37,39,41	0
3	GOL	A	408	6/6	0.80	0.17	29,35,40,48	0
3	GOL	A	412	6/6	0.81	0.15	31,42,44,45	0
3	GOL	B	410	6/6	0.82	0.12	20,39,42,43	0
3	GOL	B	405[A]	6/6	0.83	0.12	14,18,18,27	6
3	GOL	B	405[B]	6/6	0.83	0.12	22,28,31,36	6
6	EDO	A	430	4/4	0.83	0.12	30,36,38,40	0
6	EDO	A	431	4/4	0.83	0.13	17,23,29,31	0
3	GOL	B	407	6/6	0.84	0.12	28,37,39,48	0
3	GOL	B	411	6/6	0.84	0.11	26,32,35,40	0
6	EDO	A	418	4/4	0.85	0.18	15,24,30,31	0
6	EDO	A	428	4/4	0.85	0.11	34,35,36,37	0
3	GOL	A	413	6/6	0.85	0.13	29,38,42,43	0
7	PEG	A	433	7/7	0.85	0.14	18,21,32,38	0
4	CAC	A	416	5/5	0.86	0.26	33,35,43,44	0
3	GOL	B	408	6/6	0.86	0.13	27,41,42,43	0
3	GOL	A	409	6/6	0.86	0.12	23,25,30,38	0
6	EDO	B	420	4/4	0.86	0.11	27,31,32,33	0
3	GOL	A	411	6/6	0.87	0.11	25,41,44,52	0
6	EDO	B	417	4/4	0.87	0.17	17,23,23,32	0
3	GOL	A	403	6/6	0.87	0.11	22,22,25,30	0
6	EDO	A	423	4/4	0.87	0.11	20,27,28,35	0
6	EDO	A	422	4/4	0.88	0.13	31,32,36,37	0
7	PEG	B	427	7/7	0.88	0.10	20,25,26,26	0
6	EDO	B	423	4/4	0.89	0.11	22,29,34,35	0

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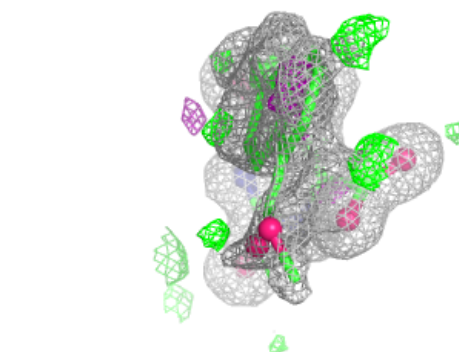
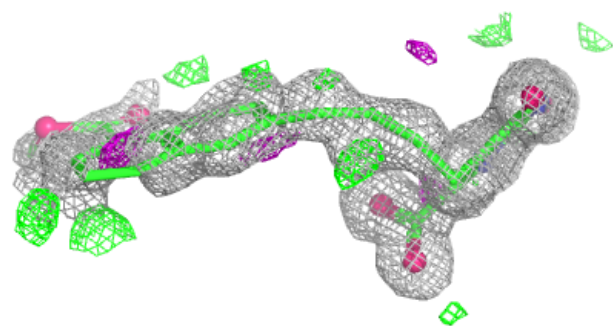
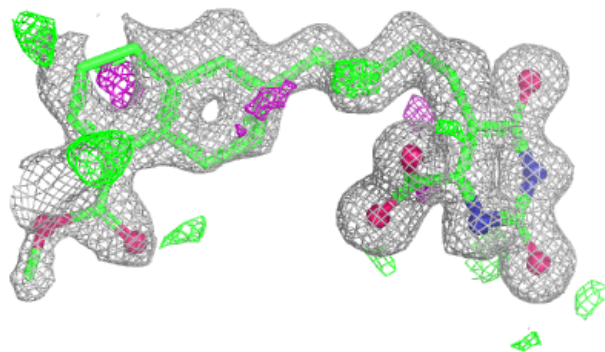
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	GOL	B	406	6/6	0.89	0.11	16,20,21,23	0
6	EDO	B	426	4/4	0.89	0.12	25,31,33,35	0
6	EDO	A	420	4/4	0.89	0.09	27,28,30,35	0
6	EDO	A	424	4/4	0.89	0.11	30,30,37,40	0
8	NCO	A	435[A]	7/7	0.89	0.25	16,26,28,29	7
8	NCO	A	435[B]	7/7	0.89	0.25	14,25,29,30	7
3	GOL	A	404	6/6	0.90	0.12	19,23,33,33	0
3	GOL	B	404	6/6	0.90	0.10	22,23,24,25	0
3	GOL	A	405	6/6	0.90	0.10	19,24,29,31	0
4	CAC	A	415	5/5	0.91	0.26	11,18,21,21	0
6	EDO	B	425	4/4	0.92	0.23	18,21,21,24	0
6	EDO	A	421	4/4	0.92	0.10	22,28,33,34	0
3	GOL	A	402[B]	6/6	0.93	0.07	8,11,11,11	6
2	W87	B	401[A]	29/29	0.93	0.10	5,11,27,29	29
2	W87	B	401[B]	29/29	0.93	0.10	5,9,24,29	29
3	GOL	A	402[A]	6/6	0.93	0.07	8,9,10,10	6
6	EDO	B	419	4/4	0.94	0.20	19,20,22,23	0
8	NCO	A	434	7/7	0.94	0.32	7,14,18,19	0
7	PEG	A	432	7/7	0.95	0.11	11,23,26,30	0
4	CAC	B	414	5/5	0.95	0.20	10,16,19,19	0
2	W87	A	401	29/29	0.96	0.09	5,16,32,34	0
3	GOL	B	402	6/6	0.96	0.07	15,15,18,18	0
5	FMN	A	417	31/31	0.99	0.03	3,4,6,6	0
5	FMN	B	416	31/31	0.99	0.03	3,4,6,6	0

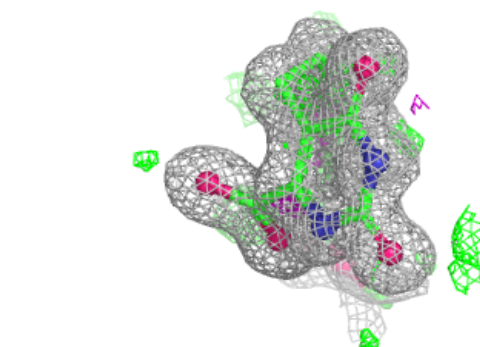
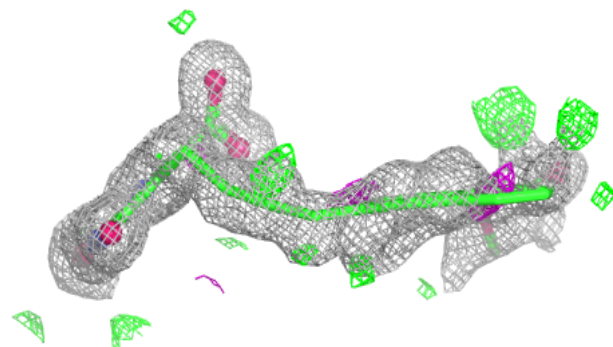
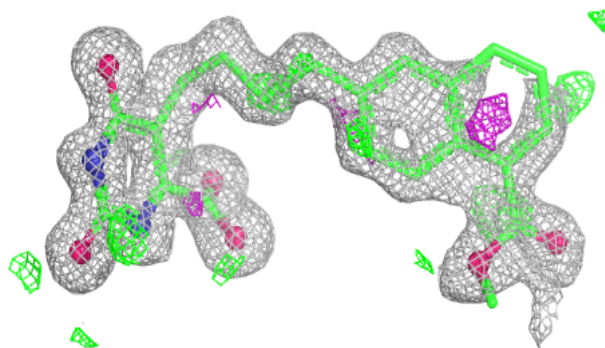
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around W87 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)

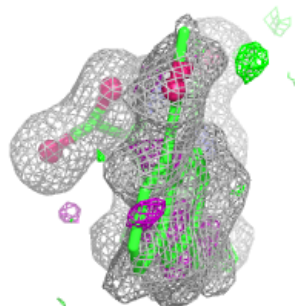
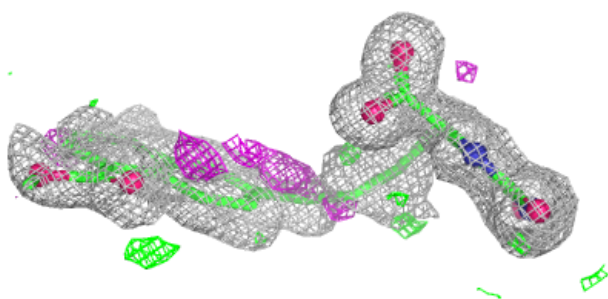
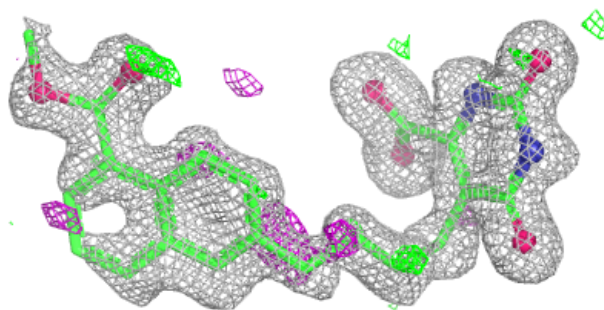
**Electron density around W87 B 401 (B):**

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



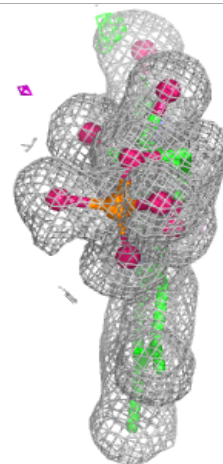
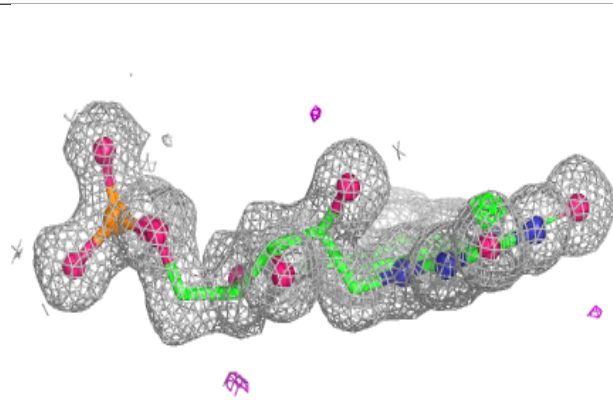
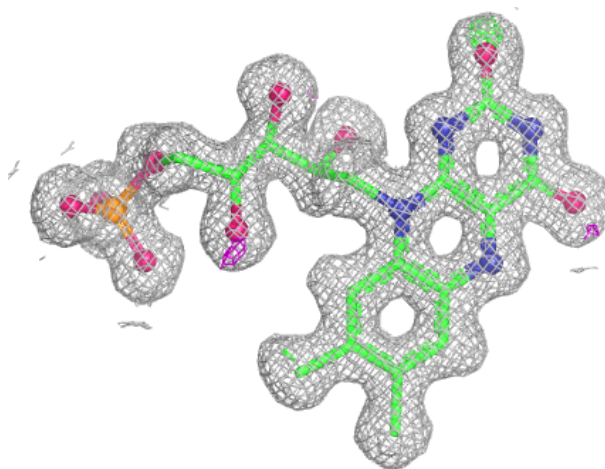
Electron density around W87 A 401:

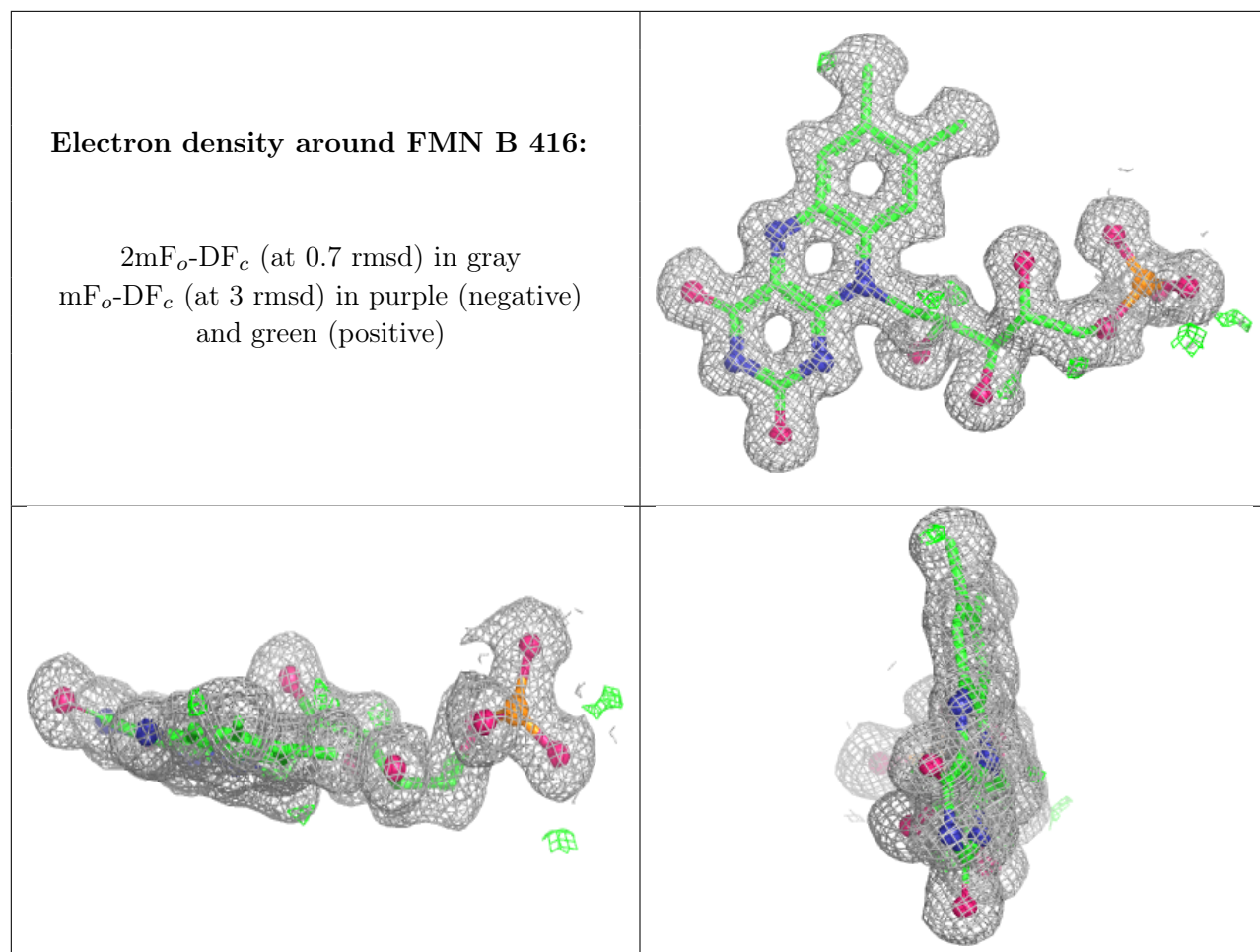
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around FMN A 417:

$2mF_o-DF_c$ (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.