



wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 2, 2023 – 08:56 PM EDT

PDB ID : 3W88
Title : Structure of Trypanosoma cruzi dihydroorotate dehydrogenase in complex with SH-1-200
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 : 1.40 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

<http://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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)

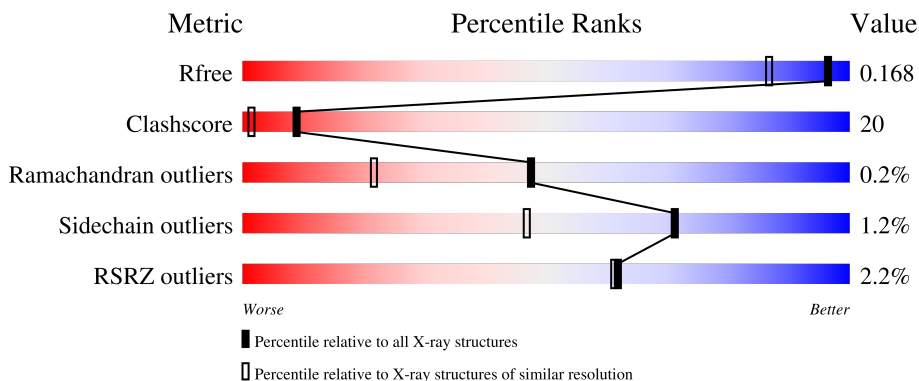
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.40 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}	130704	1714 (1.40-1.40)
Clashscore	141614	1812 (1.40-1.40)
Ramachandran outliers	138981	1763 (1.40-1.40)
Sidechain outliers	138945	1762 (1.40-1.40)
RSRZ outliers	127900	1674 (1.40-1.40)

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	 3% 75% 21%
1	B	314	 2% 80% 17%

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

Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
 Validation Pipeline (wwPDB-VP) : 2.36

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	B	412	-	-	X	-
6	EDO	A	423	-	-	X	-
6	EDO	A	427	-	-	-	X
6	EDO	A	433	-	-	X	-
6	EDO	A	434	-	-	X	-
6	EDO	A	435	-	-	X	X
6	EDO	B	416	-	-	X	-
6	EDO	B	418	-	-	X	-
6	EDO	B	420	-	-	-	X
6	EDO	B	424	-	-	X	-
7	PEG	A	437[A]	-	-	X	-
7	PEG	A	437[B]	-	-	X	-
7	PEG	A	438	-	-	X	-
7	PEG	A	439	-	-	X	-
7	PEG	A	440	-	-	X	-
7	PEG	B	431[A]	-	-	-	X
7	PEG	B	431[B]	-	-	-	X
7	PEG	B	432	-	-	X	-
7	PEG	B	433	-	-	X	-

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 6466 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

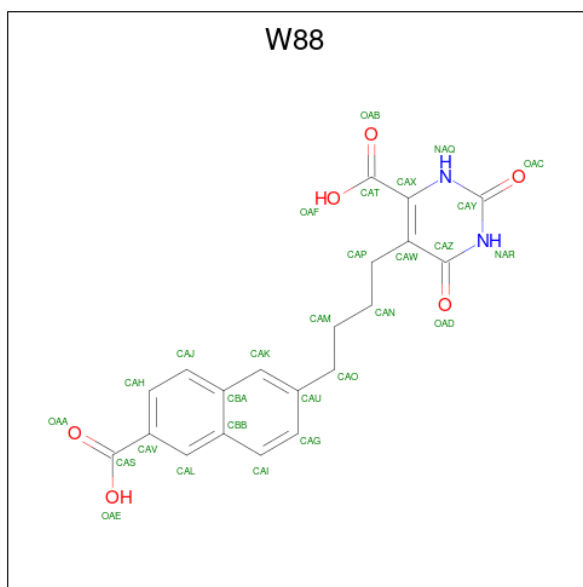
- Molecule 1 is a protein called Dihydroorotate dehydrogenase (fumarate).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	314	2554	1629	427	479	19	0	19	0
1	B	314	2533	1609	427	478	19	0	17	0

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-(6-carboxynaphthalen-2-yl)butyl]-2,6-dioxo-1,2,3,6-tetrahydropyrimidine-4-carboxylic acid (three-letter code: W88) (formula: C₂₀H₁₈N₂O₆).



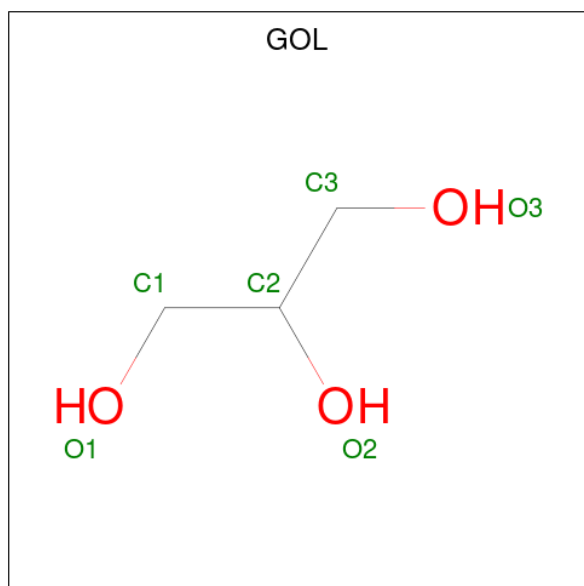
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	28	20	2	6	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	B	1	56	40	4	12	0	1

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



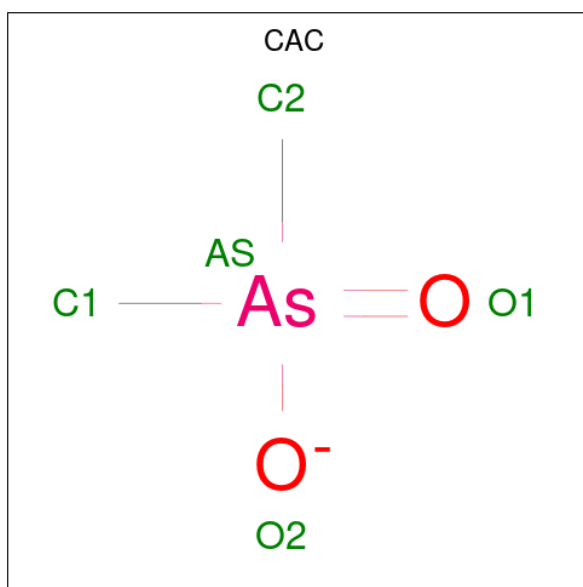
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
3	A	1	12	6	6	0	1
3	A	1	6	3	3	0	0
3	A	1	6	3	3	0	0
3	A	1	6	3	3	0	0
3	A	1	6	3	3	0	0
3	A	1	12	6	6	0	1
3	A	1	6	3	3	0	0
3	A	1	6	3	3	0	0
3	A	1	6	3	3	0	0
3	A	1	6	3	3	0	0

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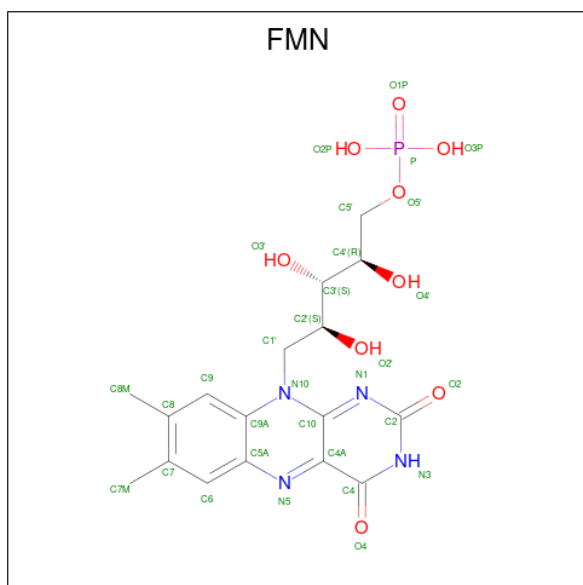
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 6	C 3	O 3	0	0
3	A	1	Total 6	C 3	O 3	0	0
3	A	1	Total 6	C 3	O 3	0	0
3	B	1	Total 6	C 3	O 3	0	0
3	B	1	Total 6	C 3	O 3	0	0
3	B	1	Total 12	C 6	O 6	0	1
3	B	1	Total 6	C 3	O 3	0	0
3	B	1	Total 6	C 3	O 3	0	0
3	B	1	Total 6	C 3	O 3	0	0
3	B	1	Total 6	C 3	O 3	0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

- Molecule 4 is CACODYLATE ION (three-letter code: CAC) (formula: C₂H₆AsO₂).



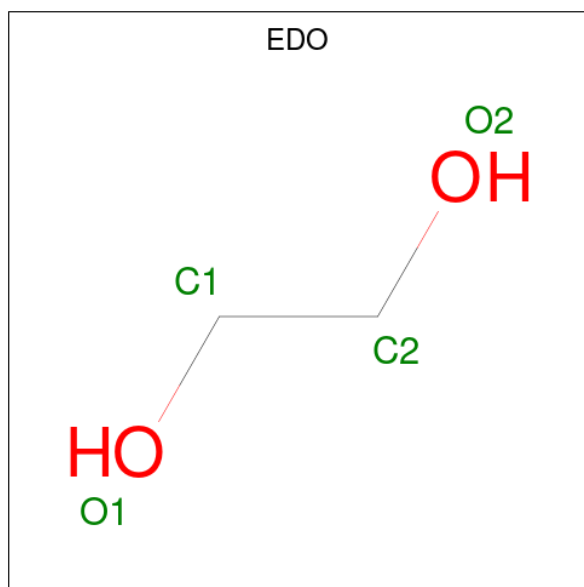
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	As	C	O		
4	A	1	5	1	2	2	0	0
4	A	1	5	1	2	2	0	0
4	B	1	5	1	2	2	0	0
4	B	1	5	1	2	2	0	0

- Molecule 5 is FLAVIN MONONUCLEOTIDE (three-letter code: 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 (three-letter code: 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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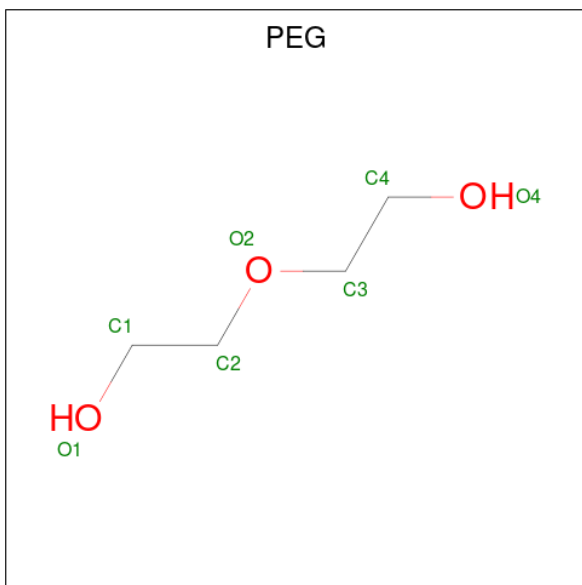
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		
6	B	1	Total	C	O	0	0
			4	2	2		
6	B	1	Total	C	O	0	0
			4	2	2		
6	B	1	Total	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		
6	B	1	Total	C	O	0	0
			4	2	2		

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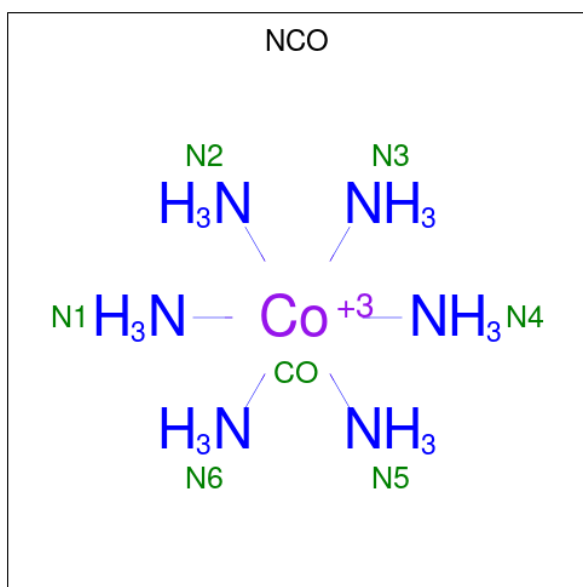
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total C O 4 2 2	0	0
6	B	1	Total C O 4 2 2	0	0

- Molecule 7 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C O 7 4 3	0	0
7	A	1	Total C O 14 8 6	0	1
7	A	1	Total C O 7 4 3	0	0
7	A	1	Total C O 7 4 3	0	0
7	A	1	Total C O 7 4 3	0	0
7	B	1	Total C O 14 8 6	0	1
7	B	1	Total C O 7 4 3	0	0
7	B	1	Total C O 7 4 3	0	0

- Molecule 8 is COBALT HEXAMMINE(III) (three-letter code: NCO) (formula: CoH₁₈N₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	Co	N	0	0
			7	1	6		
8	A	1	Total	Co	N	0	1
			14	2	12		

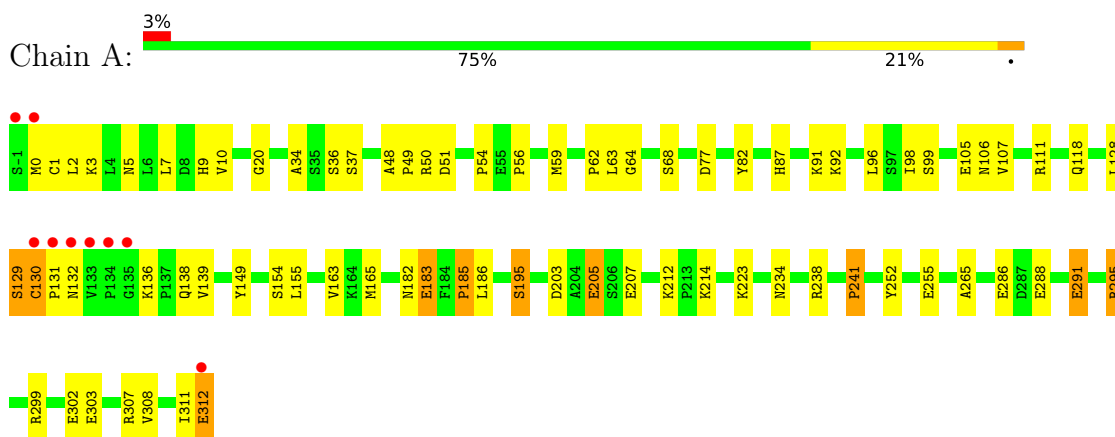
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	371	Total	O	0	10
			381	381		
9	B	440	Total	O	0	7
			447	447		

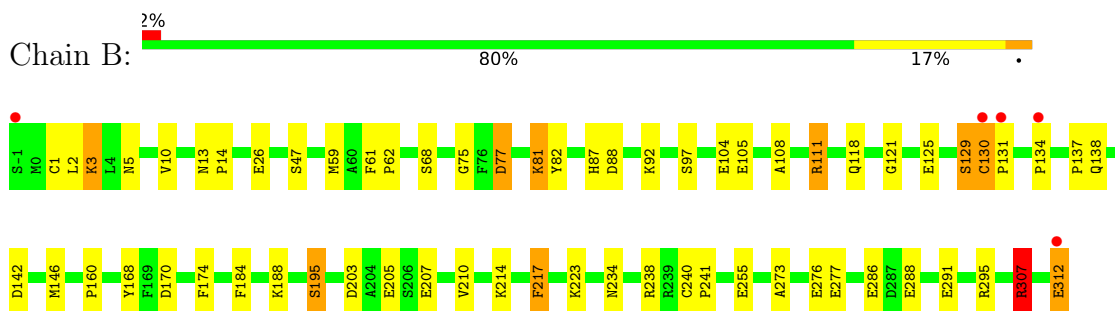
3 Residue-property plots [i](#)

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	67.97Å 71.52Å 129.54Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	36.96 – 1.40 36.96 – 1.40	Depositor EDS
% Data completeness (in resolution range)	95.1 (36.96-1.40) 95.1 (36.96-1.40)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.93 (at 1.40Å)	Xtrriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.139 , 0.166 0.143 , 0.168	Depositor DCC
R_{free} test set	5941 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	8.3	Xtrriage
Anisotropy	0.066	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 50.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.006 for k,h,-l	Xtrriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	6466	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 26.50 % 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 2.6031e-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: EDO, GOL, NCO, PEG, FMN, W88, CAC

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	1.62	29/2606 (1.1%)	1.21	6/3524 (0.2%)
1	B	1.52	27/2585 (1.0%)	1.29	26/3496 (0.7%)
All	All	1.57	56/5191 (1.1%)	1.25	32/7020 (0.5%)

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

The worst 5 of 56 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	130[A]	CYS	C-N	18.62	1.69	1.34
1	A	130[B]	CYS	C-N	18.62	1.69	1.34
1	B	205[A]	GLU	CD-OE2	-11.18	1.13	1.25
1	B	205[B]	GLU	CD-OE2	-11.18	1.13	1.25
1	B	105	GLU	CD-OE1	-10.49	1.14	1.25

The worst 5 of 32 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	3	LYS	CD-CE-NZ	14.44	144.92	111.70
1	A	129	SER	O-C-N	-10.41	106.03	122.70
1	B	129	SER	O-C-N	-9.33	107.77	122.70
1	B	130[A]	CYS	CA-CB-SG	9.05	130.28	114.00
1	B	130[B]	CYS	CA-CB-SG	9.05	130.28	114.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	129	SER	Mainchain

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	2554	0	2540	115	0
1	B	2533	0	2512	62	0
2	A	28	0	16	1	0
2	B	56	0	32	8	0
3	A	90	0	119	6	0
3	B	72	0	95	12	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	72	0	107	34	0
6	B	60	0	88	31	0
7	A	42	0	59	38	0
7	B	28	0	40	18	0
8	A	21	0	0	2	0
9	A	381	0	0	25	0
9	B	447	0	0	28	0
All	All	6466	0	5646	230	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 20.

The worst 5 of 230 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	1.68	1.54
1:A:130[A]:CYS:C	1:A:131:PRO:N	1.69	1.42
1:A:130[B]:CYS:C	1:A:131:PRO:N	1.73	1.39

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1:CYS:HB2	7:A:437[B]:PEG:H22	1.33	1.11
2:B:401[A]:W88:CAI	7:B:433:PEG:H22	1.81	1.10

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	330/314 (105%)	323 (98%)	6 (2%)	1 (0%)	41	18
1	B	329/314 (105%)	318 (97%)	11 (3%)	0	100	100
All	All	659/628 (105%)	641 (97%)	17 (3%)	1 (0%)	47	21

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	0	MET

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	278/259 (107%)	274 (99%)	4 (1%)	67	40
1	B	276/259 (107%)	272 (99%)	4 (1%)	67	40
All	All	554/518 (107%)	546 (99%)	8 (1%)	71	40

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

Mol	Chain	Res	Type
1	B	312	GLU
1	B	307[B]	ARG
1	B	118	GLN
1	A	312[B]	GLU
1	B	307[A]	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	118	GLN
1	B	138	GLN
1	B	234	ASN
1	A	151	GLN
1	A	234	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

82 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
7	PEG	B	431[A]	-	6,6,6	0.57	0	5,5,5	0.39	0
6	EDO	B	428	-	3,3,3	0.60	0	2,2,2	0.13	0
3	GOL	A	407[A]	-	5,5,5	0.29	0	5,5,5	0.35	0
3	GOL	B	409	-	5,5,5	0.68	0	5,5,5	0.62	0
3	GOL	B	406	-	5,5,5	0.38	0	5,5,5	0.35	0
4	CAC	A	415	-	0,4,4	-	-	0,6,6	-	-
3	GOL	A	402[A]	-	5,5,5	1.13	0	5,5,5	0.73	0
6	EDO	A	418	-	3,3,3	1.15	0	2,2,2	0.66	0
6	EDO	B	424	-	3,3,3	0.94	0	2,2,2	1.76	1 (50%)
6	EDO	A	419	-	3,3,3	0.55	0	2,2,2	0.38	0
3	GOL	A	413	-	5,5,5	0.77	0	5,5,5	0.97	0
7	PEG	A	440	-	6,6,6	0.50	0	5,5,5	0.97	0
6	EDO	B	416	-	3,3,3	1.43	0	2,2,2	1.49	0
7	PEG	A	436	-	6,6,6	1.02	1 (16%)	5,5,5	1.59	2 (40%)
2	W88	B	401[B]	-	29,30,30	1.53	6 (20%)	39,42,42	1.15	4 (10%)
4	CAC	B	413	-	0,4,4	-	-	0,6,6	-	-
6	EDO	B	421	-	3,3,3	0.59	0	2,2,2	0.32	0
6	EDO	B	420	-	3,3,3	0.60	0	2,2,2	0.08	0
6	EDO	A	431	-	3,3,3	0.80	0	2,2,2	0.44	0
6	EDO	A	420	-	3,3,3	0.88	0	2,2,2	1.27	0
3	GOL	B	411	-	5,5,5	0.67	0	5,5,5	0.91	0
6	EDO	B	429	-	3,3,3	0.57	0	2,2,2	0.27	0
6	EDO	B	417	-	3,3,3	0.25	0	2,2,2	1.18	0
4	CAC	A	416	-	0,4,4	-	-	0,6,6	-	-
7	PEG	B	433	-	6,6,6	0.41	0	5,5,5	0.96	0
6	EDO	A	433	-	3,3,3	1.18	0	2,2,2	1.10	0
2	W88	B	401[A]	-	29,30,30	1.76	5 (17%)	39,42,42	1.33	7 (17%)
4	CAC	B	414	-	0,4,4	-	-	0,6,6	-	-
3	GOL	A	404	-	5,5,5	0.47	0	5,5,5	0.52	0
5	FMN	A	417	-	33,33,33	1.32	3 (9%)	48,50,50	1.29	6 (12%)
5	FMN	B	415	-	33,33,33	1.39	6 (18%)	48,50,50	1.20	5 (10%)
8	NCO	A	442[B]	-	6,6,6	1.17	0	-	-	-
6	EDO	B	422	-	3,3,3	0.35	0	2,2,2	0.08	0
3	GOL	B	404[B]	-	5,5,5	0.46	0	5,5,5	1.44	0
3	GOL	A	408	-	5,5,5	0.40	0	5,5,5	0.55	0
3	GOL	A	405	-	5,5,5	1.38	1 (20%)	5,5,5	1.73	1 (20%)
3	GOL	B	408	-	5,5,5	1.12	1 (20%)	5,5,5	1.03	0
8	NCO	A	441	-	6,6,6	2.77	6 (100%)	-	-	-
7	PEG	A	437[B]	-	6,6,6	0.67	0	5,5,5	1.48	1 (20%)
7	PEG	A	439	-	6,6,6	0.72	0	5,5,5	1.79	1 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	EDO	A	423	-	3,3,3	0.75	0	2,2,2	1.10	0
8	NCO	A	442[A]	-	6,6,6	0.89	0	-		
6	EDO	A	425	-	3,3,3	0.84	0	2,2,2	0.19	0
3	GOL	B	404[A]	-	5,5,5	0.96	0	5,5,5	0.76	0
3	GOL	B	405	-	5,5,5	0.95	0	5,5,5	1.40	1 (20%)
3	GOL	A	414	-	5,5,5	0.48	0	5,5,5	0.28	0
6	EDO	B	427	-	3,3,3	0.70	0	2,2,2	0.69	0
3	GOL	A	403	-	5,5,5	0.90	0	5,5,5	1.15	0
3	GOL	A	412	-	5,5,5	0.81	0	5,5,5	1.41	1 (20%)
6	EDO	A	434	-	3,3,3	0.50	0	2,2,2	0.93	0
6	EDO	B	418	-	3,3,3	0.80	0	2,2,2	0.87	0
2	W88	A	401	-	29,30,30	1.76	6 (20%)	39,42,42	1.31	5 (12%)
3	GOL	A	411	-	5,5,5	0.84	0	5,5,5	0.81	0
6	EDO	B	423	-	3,3,3	0.82	0	2,2,2	1.06	0
6	EDO	A	435	-	3,3,3	0.89	0	2,2,2	0.53	0
7	PEG	A	437[A]	-	6,6,6	0.80	0	5,5,5	1.60	1 (20%)
7	PEG	A	438	-	6,6,6	0.36	0	5,5,5	1.44	0
6	EDO	A	426	-	3,3,3	0.55	0	2,2,2	0.35	0
6	EDO	B	425	-	3,3,3	1.01	0	2,2,2	0.85	0
3	GOL	B	403	-	5,5,5	1.30	1 (20%)	5,5,5	1.10	0
6	EDO	A	429	-	3,3,3	0.89	0	2,2,2	0.44	0
7	PEG	B	431[B]	-	6,6,6	0.53	0	5,5,5	0.82	0
6	EDO	A	430	-	3,3,3	0.66	0	2,2,2	0.60	0
7	PEG	B	432	-	6,6,6	1.29	0	5,5,5	1.68	2 (40%)
3	GOL	A	407[B]	-	5,5,5	0.37	0	5,5,5	0.67	0
3	GOL	B	407	-	5,5,5	0.66	0	5,5,5	0.78	0
3	GOL	A	402[B]	-	5,5,5	1.19	0	5,5,5	1.28	1 (20%)
3	GOL	B	410	-	5,5,5	0.55	0	5,5,5	1.43	1 (20%)
3	GOL	B	402	-	5,5,5	0.61	0	5,5,5	1.06	0
6	EDO	B	430	-	3,3,3	0.86	0	2,2,2	0.46	0
3	GOL	A	406	-	5,5,5	0.82	0	5,5,5	1.47	2 (40%)
6	EDO	A	421	-	3,3,3	0.34	0	2,2,2	1.37	0
3	GOL	B	412	-	5,5,5	0.64	0	5,5,5	0.91	0
6	EDO	A	422	-	3,3,3	1.04	0	2,2,2	0.50	0
6	EDO	A	424	-	3,3,3	0.55	0	2,2,2	0.42	0
3	GOL	A	410	-	5,5,5	0.90	0	5,5,5	1.36	1 (20%)
6	EDO	B	426	-	3,3,3	0.51	0	2,2,2	1.15	0
6	EDO	A	432	-	3,3,3	0.80	0	2,2,2	0.72	0
6	EDO	B	419	-	3,3,3	0.77	0	2,2,2	0.82	0
6	EDO	A	427	-	3,3,3	0.56	0	2,2,2	0.05	0
6	EDO	A	428	-	3,3,3	0.61	0	2,2,2	0.41	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	GOL	A	409	-	5,5,5	0.78	0	5,5,5	1.17	1 (20%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	PEG	B	431[A]	-	-	3/4/4/4	-
3	GOL	B	408	-	-	4/4/4/4	-
6	EDO	A	435	-	-	1/1/1/1	-
7	PEG	A	437[A]	-	-	4/4/4/4	-
6	EDO	B	428	-	-	0/1/1/1	-
3	GOL	A	407[A]	-	-	1/4/4/4	-
3	GOL	B	409	-	-	0/4/4/4	-
6	EDO	A	420	-	-	1/1/1/1	-
3	GOL	B	411	-	-	2/4/4/4	-
6	EDO	A	426	-	-	1/1/1/1	-
6	EDO	B	425	-	-	0/1/1/1	-
6	EDO	B	429	-	-	1/1/1/1	-
7	PEG	A	438	-	-	3/4/4/4	-
3	GOL	B	403	-	-	0/4/4/4	-
3	GOL	B	406	-	-	2/4/4/4	-
3	GOL	A	402[A]	-	-	0/4/4/4	-
6	EDO	A	418	-	-	1/1/1/1	-
6	EDO	A	429	-	-	1/1/1/1	-
6	EDO	B	417	-	-	0/1/1/1	-
7	PEG	B	431[B]	-	-	3/4/4/4	-
6	EDO	B	424	-	-	1/1/1/1	-
6	EDO	A	430	-	-	1/1/1/1	-
7	PEG	A	437[B]	-	-	3/4/4/4	-
7	PEG	A	439	-	-	2/4/4/4	-
7	PEG	B	432	-	-	3/4/4/4	-
3	GOL	A	407[B]	-	-	4/4/4/4	-
6	EDO	A	423	-	-	1/1/1/1	-
3	GOL	B	407	-	-	2/4/4/4	-
6	EDO	A	433	-	-	1/1/1/1	-
6	EDO	A	419	-	-	0/1/1/1	-
7	PEG	B	433	-	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	A	413	-	-	4/4/4/4	-
2	W88	B	401[A]	-	-	8/15/15/15	0/3/3/3
7	PEG	A	440	-	-	3/4/4/4	-
3	GOL	A	402[B]	-	-	0/4/4/4	-
3	GOL	A	408	-	-	0/4/4/4	-
3	GOL	B	410	-	-	2/4/4/4	-
3	GOL	B	402	-	-	2/4/4/4	-
6	EDO	B	416	-	-	0/1/1/1	-
6	EDO	A	425	-	-	0/1/1/1	-
3	GOL	A	404	-	-	0/4/4/4	-
7	PEG	A	436	-	-	2/4/4/4	-
5	FMN	A	417	-	-	1/18/18/18	0/3/3/3
5	FMN	B	415	-	-	1/18/18/18	0/3/3/3
6	EDO	B	430	-	-	1/1/1/1	-
3	GOL	A	406	-	-	0/4/4/4	-
3	GOL	B	404[A]	-	-	0/4/4/4	-
6	EDO	A	421	-	-	1/1/1/1	-
3	GOL	B	405	-	-	1/4/4/4	-
3	GOL	B	412	-	-	2/4/4/4	-
6	EDO	A	422	-	-	1/1/1/1	-
6	EDO	A	424	-	-	1/1/1/1	-
2	W88	B	401[B]	-	-	3/15/15/15	0/3/3/3
3	GOL	A	414	-	-	2/4/4/4	-
6	EDO	B	421	-	-	1/1/1/1	-
3	GOL	A	410	-	-	1/4/4/4	-
6	EDO	B	420	-	-	0/1/1/1	-
6	EDO	B	426	-	-	0/1/1/1	-
6	EDO	B	427	-	-	1/1/1/1	-
3	GOL	A	403	-	-	0/4/4/4	-
3	GOL	A	412	-	-	0/4/4/4	-
3	GOL	B	404[B]	-	-	4/4/4/4	-
6	EDO	A	434	-	-	1/1/1/1	-
6	EDO	A	431	-	-	0/1/1/1	-
6	EDO	B	422	-	-	1/1/1/1	-
6	EDO	A	432	-	-	1/1/1/1	-
6	EDO	B	418	-	-	1/1/1/1	-
6	EDO	B	419	-	-	1/1/1/1	-
6	EDO	A	428	-	-	0/1/1/1	-
2	W88	A	401	-	-	4/15/15/15	0/3/3/3
6	EDO	A	427	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	A	411	-	-	4/4/4/4	-
3	GOL	A	405	-	-	3/4/4/4	-
6	EDO	B	423	-	-	0/1/1/1	-
3	GOL	A	409	-	-	1/4/4/4	-

The worst 5 of 36 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401[A]	W88	CAV-CAS	-6.10	1.36	1.49
5	A	417	FMN	C4-N3	-4.79	1.29	1.38
2	A	401	W88	CAL-CAV	4.16	1.44	1.37
5	B	415	FMN	C4-N3	-3.81	1.31	1.38
2	B	401[B]	W88	CAV-CAS	-3.60	1.41	1.49

The worst 5 of 44 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	439	PEG	O2-C2-C1	-3.52	94.60	110.07
5	A	417	FMN	C4-C4A-N5	3.51	123.22	118.23
7	A	437[A]	PEG	C3-O2-C2	3.51	128.48	113.29
3	A	405	GOL	O3-C3-C2	3.34	126.20	110.20
5	B	415	FMN	C5A-C6-C7	2.95	126.13	120.71

There are no chirality outliers.

5 of 106 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	W88	OAF-CAT-CAX-NAQ
2	B	401[A]	W88	OAF-CAT-CAX-NAQ
2	B	401[B]	W88	OAF-CAT-CAX-NAQ
3	A	405	GOL	O1-C1-C2-C3
3	A	405	GOL	C1-C2-C3-O3

There are no ring outliers.

53 monomers are involved in 144 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	409	GOL	1	0
4	A	415	CAC	1	0
3	A	402[A]	GOL	1	0

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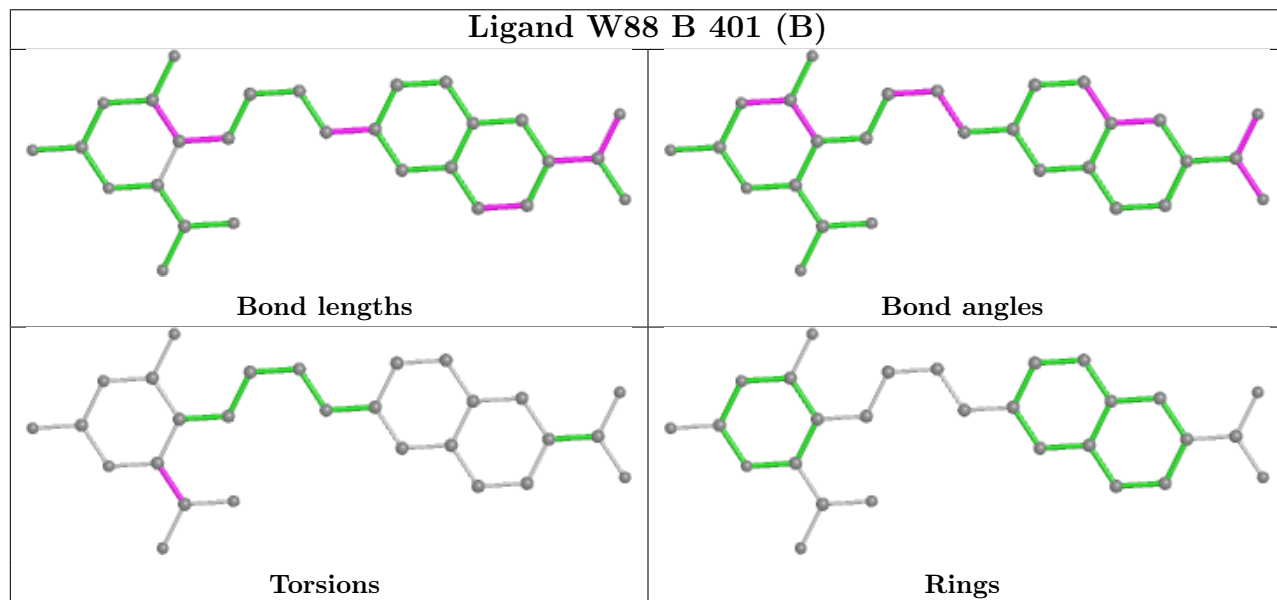
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	418	EDO	3	0
6	B	424	EDO	4	0
3	A	413	GOL	1	0
7	A	440	PEG	10	0
6	B	416	EDO	6	0
7	A	436	PEG	3	0
2	B	401[B]	W88	3	0
6	B	421	EDO	2	0
6	B	420	EDO	1	0
6	A	431	EDO	1	0
6	A	420	EDO	3	0
6	B	429	EDO	3	0
4	A	416	CAC	1	0
7	B	433	PEG	6	0
6	A	433	EDO	4	0
2	B	401[A]	W88	5	0
5	A	417	FMN	1	0
8	A	442[B]	NCO	1	0
6	B	422	EDO	1	0
3	B	408	GOL	2	0
7	A	437[B]	PEG	7	0
7	A	439	PEG	4	0
6	A	423	EDO	4	0
8	A	442[A]	NCO	1	0
6	A	425	EDO	1	0
3	A	414	GOL	1	0
6	B	427	EDO	1	0
3	A	403	GOL	1	0
6	A	434	EDO	6	0
6	B	418	EDO	4	0
2	A	401	W88	1	0
3	A	411	GOL	1	0
6	B	423	EDO	1	0
6	A	435	EDO	7	0
7	A	437[A]	PEG	9	0
7	A	438	PEG	12	0
6	A	426	EDO	1	0
6	B	425	EDO	1	0
7	B	431[B]	PEG	3	0
7	B	432	PEG	9	0
3	B	410	GOL	2	0
3	B	402	GOL	2	0

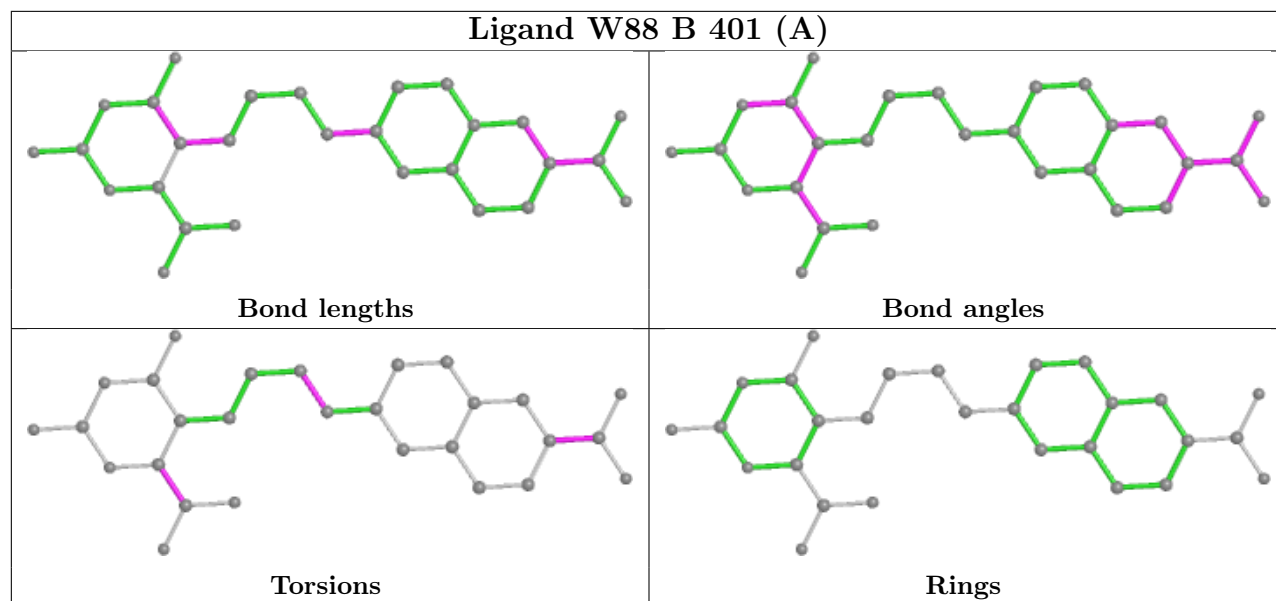
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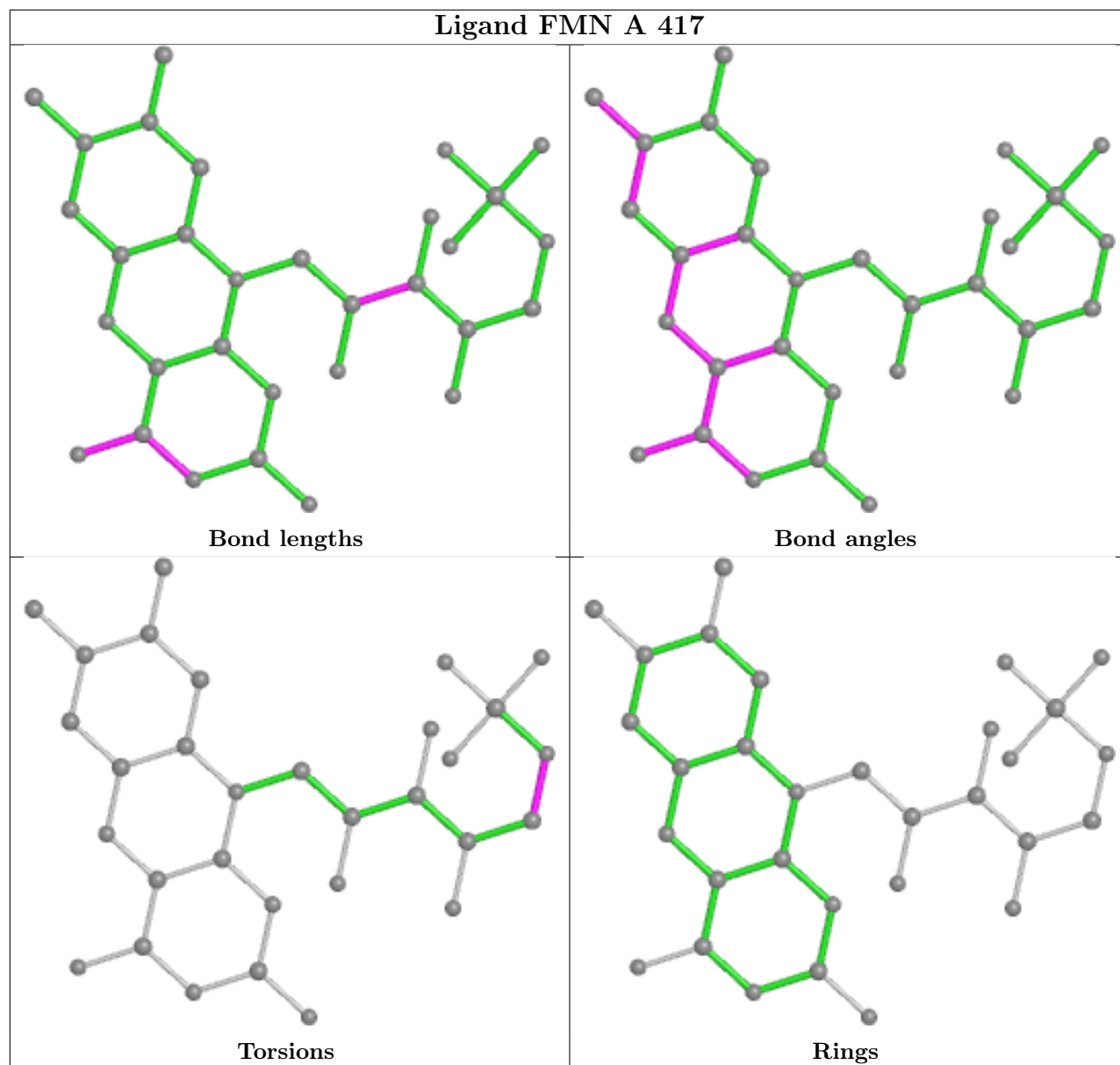
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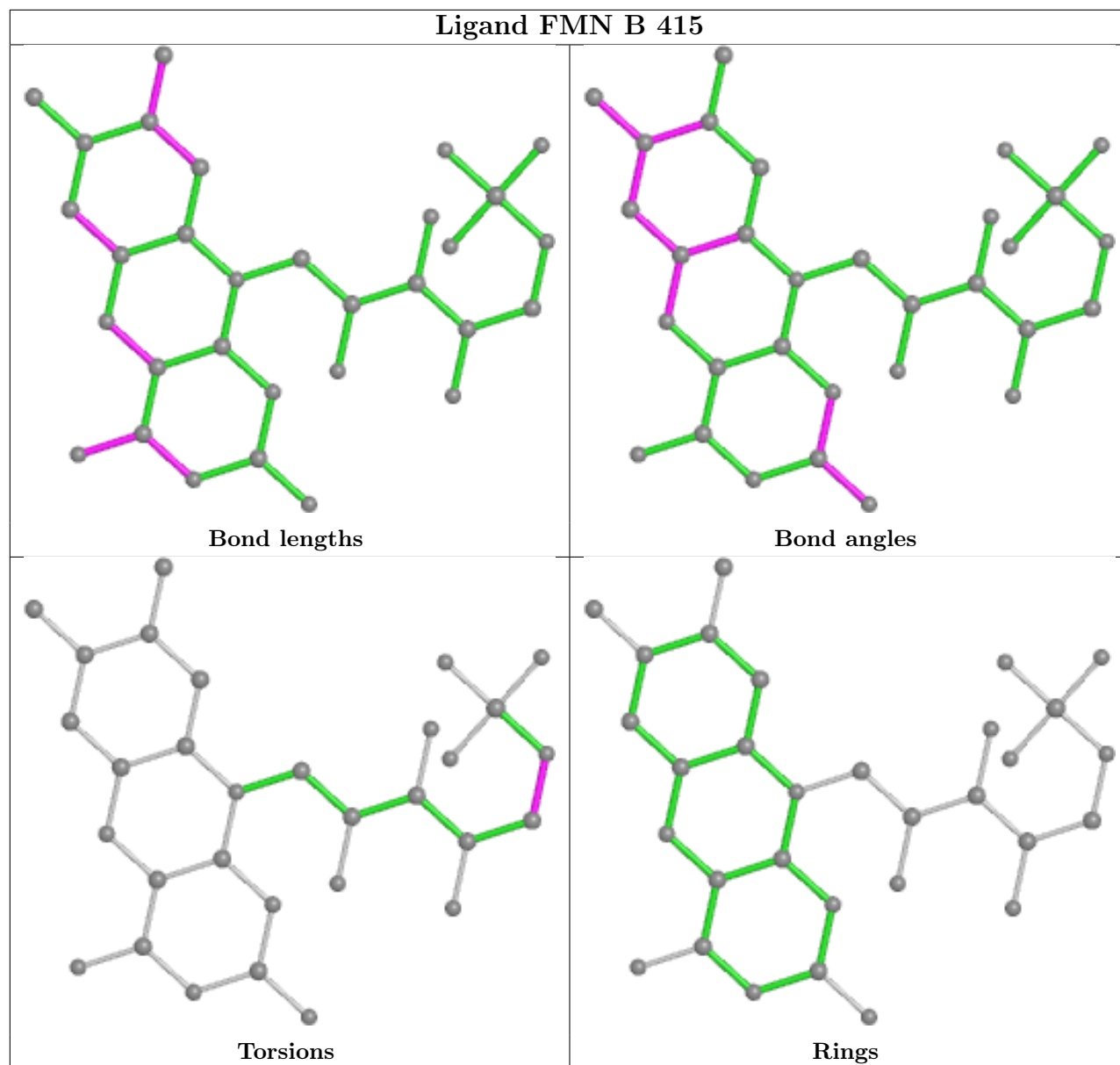
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	430	EDO	2	0
3	A	406	GOL	1	0
3	B	412	GOL	5	0
6	A	424	EDO	1	0
6	B	426	EDO	3	0
6	A	432	EDO	1	0
6	B	419	EDO	2	0
6	A	427	EDO	2	0

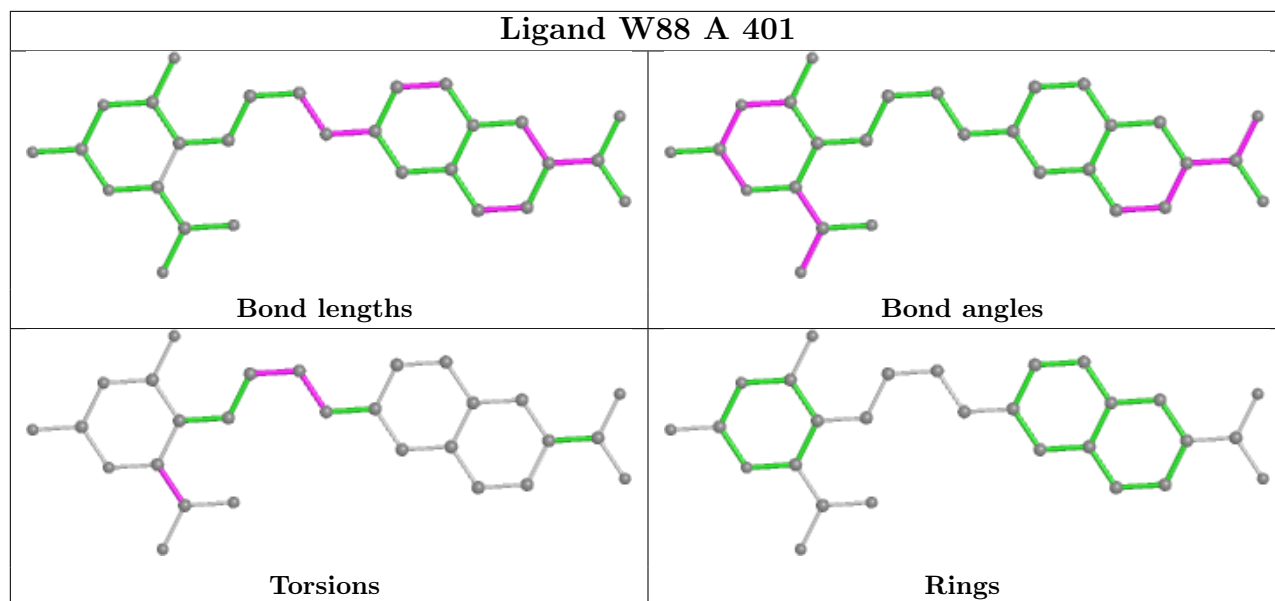
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	130[B]:CYS	C	131:PRO	N	1.73
1	A	130[A]:CYS	C	131:PRO	N	1.69

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%)	-0.14	9 (2%) 51 50	4, 9, 26, 54	0
1	B	314/314 (100%)	-0.30	5 (1%) 72 71	4, 8, 20, 45	0
All	All	628/628 (100%)	-0.22	14 (2%) 62 61	4, 8, 23, 54	0

The worst 5 of 14 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	131	PRO	7.4
1	A	133	VAL	7.2
1	A	-1	SER	5.7
1	A	135	GLY	5.1
1	A	134	PRO	5.1

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 monosaccharides 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(\AA^2)	Q<0.9
6	EDO	A	430	4/4	0.17	0.30	63,68,70,72	0
6	EDO	A	419	4/4	0.41	0.18	57,59,64,65	0
6	EDO	A	422	4/4	0.50	0.31	39,56,57,59	0
3	GOL	A	411	6/6	0.52	0.23	46,61,66,74	0
6	EDO	A	428	4/4	0.58	0.17	48,50,51,56	0
3	GOL	B	411	6/6	0.59	0.26	51,52,54,55	0
6	EDO	B	420	4/4	0.60	0.41	56,61,62,63	0
6	EDO	B	423	4/4	0.62	0.21	39,46,46,49	0
3	GOL	B	408	6/6	0.65	0.18	30,34,38,47	0
3	GOL	A	409	6/6	0.66	0.24	30,34,38,51	0
3	GOL	A	408	6/6	0.67	0.26	46,51,62,64	0
6	EDO	A	425	4/4	0.69	0.26	31,35,41,41	0
6	EDO	A	427	4/4	0.70	0.43	52,53,56,58	0
6	EDO	A	431	4/4	0.70	0.28	40,52,52,58	0
6	EDO	B	428	4/4	0.71	0.25	50,52,54,56	0
7	PEG	A	439	7/7	0.71	0.37	24,31,37,38	0
7	PEG	B	431[A]	7/7	0.71	0.53	61,80,102,108	7
7	PEG	B	431[B]	7/7	0.71	0.53	23,26,27,29	7
6	EDO	A	426	4/4	0.73	0.30	54,57,60,61	0
6	EDO	A	429	4/4	0.74	0.16	36,39,40,44	0
6	EDO	A	435	4/4	0.74	0.42	33,37,38,44	0
4	CAC	B	414	5/5	0.75	0.25	142,150,164,166	0
7	PEG	A	437[B]	7/7	0.77	0.23	20,21,26,27	7
3	GOL	A	414	6/6	0.77	0.24	39,50,52,56	0
6	EDO	B	430	4/4	0.77	0.31	35,37,39,44	0
7	PEG	A	437[A]	7/7	0.77	0.23	21,21,28,28	7
3	GOL	A	413	6/6	0.79	0.18	29,37,39,40	0
3	GOL	B	402	6/6	0.79	0.23	23,33,39,39	0
6	EDO	B	421	4/4	0.80	0.18	37,38,45,47	0
6	EDO	B	417	4/4	0.81	0.18	32,35,35,41	0
6	EDO	B	419	4/4	0.81	0.21	27,31,34,35	0
3	GOL	A	407[B]	6/6	0.81	0.20	20,28,29,30	6
3	GOL	A	407[A]	6/6	0.81	0.20	37,41,42,48	6
3	GOL	B	404[B]	6/6	0.82	0.18	21,26,27,28	6
6	EDO	A	432	4/4	0.82	0.17	34,40,41,42	0
3	GOL	A	403	6/6	0.82	0.12	23,23,25,29	0
3	GOL	A	406	6/6	0.82	0.18	21,27,27,30	0
3	GOL	B	404[A]	6/6	0.82	0.18	16,18,21,25	6
6	EDO	B	429	4/4	0.83	0.22	33,40,45,55	0
7	PEG	B	432	7/7	0.83	0.23	22,26,30,34	0
3	GOL	B	410	6/6	0.84	0.29	26,30,33,37	0
6	EDO	B	426	4/4	0.84	0.22	26,34,35,39	0
7	PEG	A	440	7/7	0.84	0.28	27,33,36,43	0

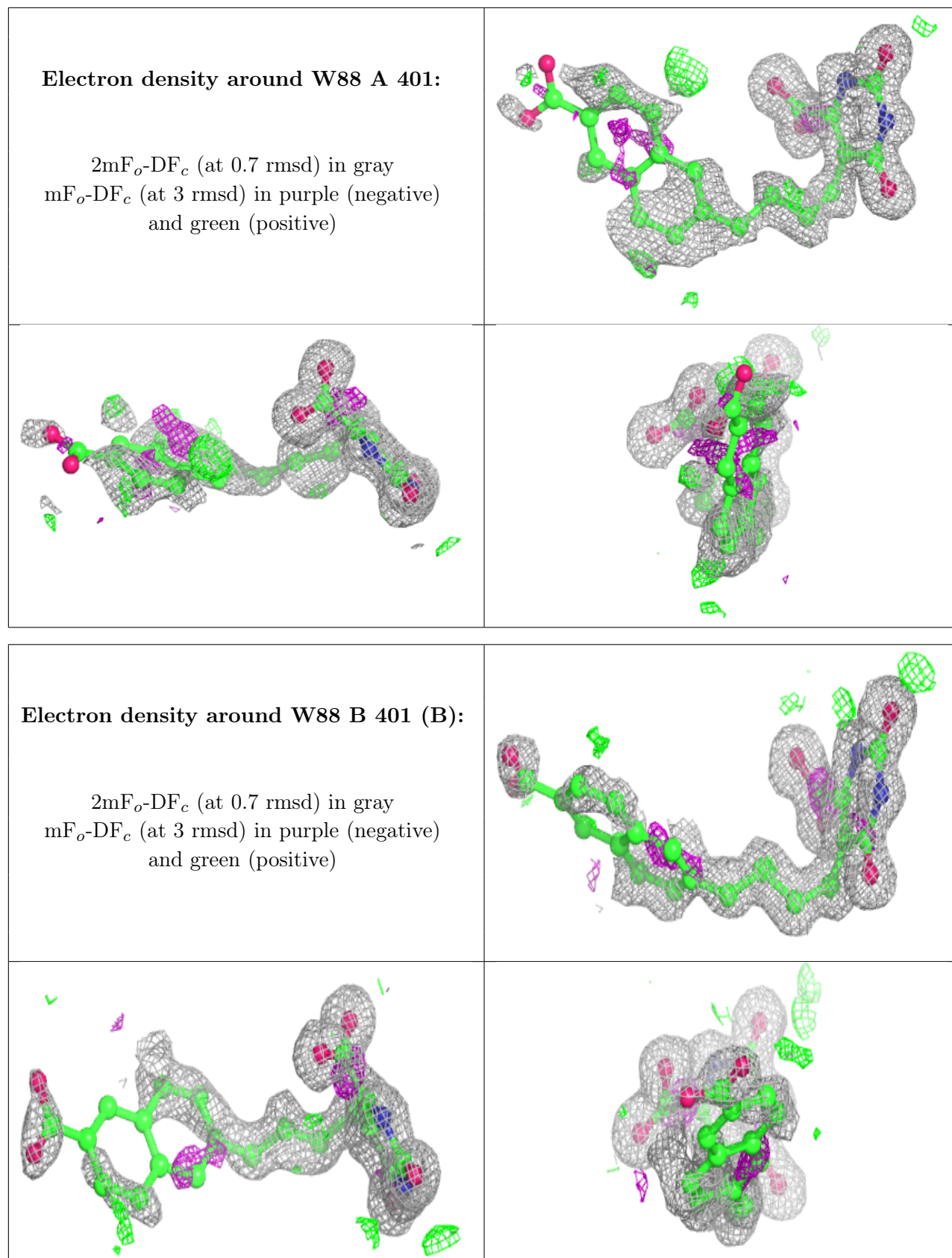
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	EDO	A	424	4/4	0.85	0.21	33,34,40,42	0
6	EDO	A	418	4/4	0.85	0.26	17,24,29,30	0
6	EDO	B	422	4/4	0.85	0.29	27,32,34,35	0
3	GOL	B	405	6/6	0.85	0.17	17,22,23,26	0
3	GOL	B	407	6/6	0.85	0.18	25,40,41,45	0
6	EDO	B	416	4/4	0.86	0.21	18,23,24,35	0
3	GOL	A	412	6/6	0.86	0.23	29,40,43,44	0
6	EDO	A	423	4/4	0.86	0.25	20,23,27,38	0
6	EDO	A	433	4/4	0.87	0.13	20,25,30,36	0
6	EDO	A	434	4/4	0.88	0.25	25,25,26,29	0
6	EDO	B	427	4/4	0.88	0.23	20,28,34,38	0
6	EDO	B	425	4/4	0.88	0.21	24,29,30,30	0
3	GOL	A	410	6/6	0.89	0.13	24,27,28,41	0
3	GOL	B	403	6/6	0.89	0.13	22,24,26,26	0
3	GOL	B	406	6/6	0.90	0.17	29,40,44,54	0
3	GOL	B	409	6/6	0.90	0.34	22,37,39,40	0
7	PEG	A	438	7/7	0.90	0.46	29,32,34,34	0
3	GOL	B	412	6/6	0.90	0.30	22,32,36,49	0
6	EDO	A	421	4/4	0.91	0.14	29,30,34,38	0
4	CAC	A	415	5/5	0.92	0.27	11,17,21,22	0
3	GOL	A	405	6/6	0.92	0.12	17,21,32,32	0
6	EDO	A	420	4/4	0.92	0.24	24,29,30,31	0
7	PEG	B	433	7/7	0.92	0.33	19,29,39,46	0
7	PEG	A	436	7/7	0.93	0.16	13,25,28,33	0
2	W88	A	401	28/28	0.94	0.14	7,22,61,70	0
4	CAC	B	413	5/5	0.95	0.23	12,16,18,20	0
2	W88	B	401[B]	28/28	0.95	0.15	6,14,26,29	28
6	EDO	B	418	4/4	0.95	0.18	19,20,22,22	0
2	W88	B	401[A]	28/28	0.95	0.15	6,13,34,36	28
3	GOL	A	404	6/6	0.95	0.07	16,18,19,22	0
4	CAC	A	416	5/5	0.95	0.33	30,34,39,43	0
8	NCO	A	442[A]	7/7	0.95	0.16	16,17,19,21	7
8	NCO	A	442[B]	7/7	0.95	0.16	15,16,18,20	7
6	EDO	B	424	4/4	0.96	0.22	16,22,22,27	0
3	GOL	A	402[A]	6/6	0.97	0.07	9,9,10,10	6
3	GOL	A	402[B]	6/6	0.97	0.07	9,10,11,12	6
5	FMN	B	415	31/31	0.98	0.07	3,4,5,6	0
5	FMN	A	417	31/31	0.99	0.07	3,4,6,6	0
8	NCO	A	441	7/7	0.99	0.09	6,6,7,7	0

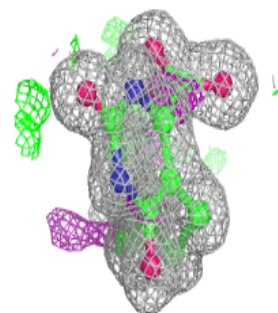
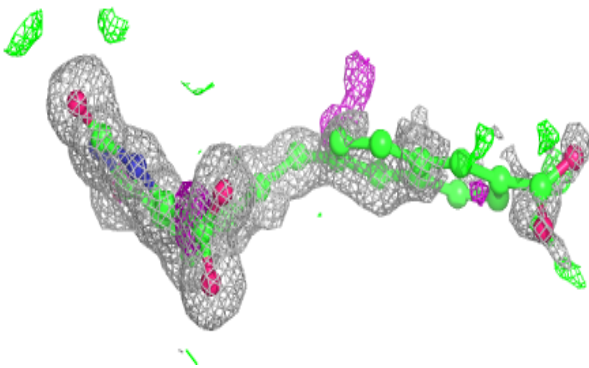
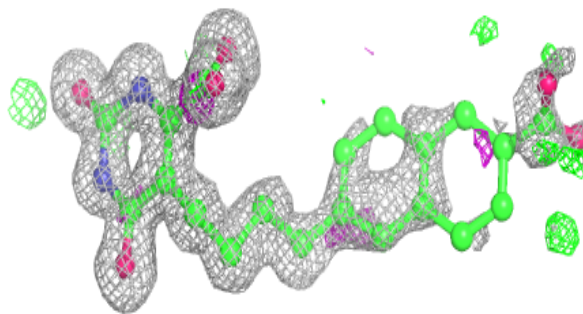
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different

orientation to approximate a three-dimensional view.



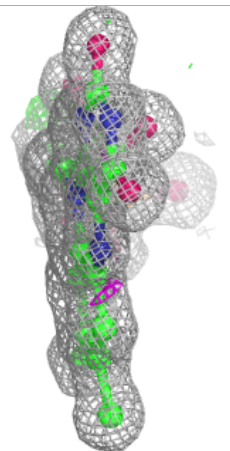
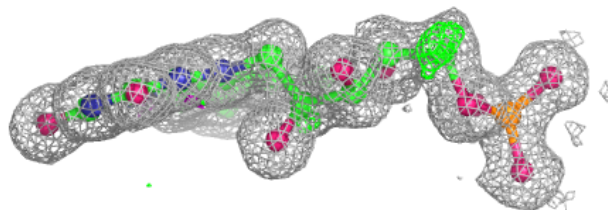
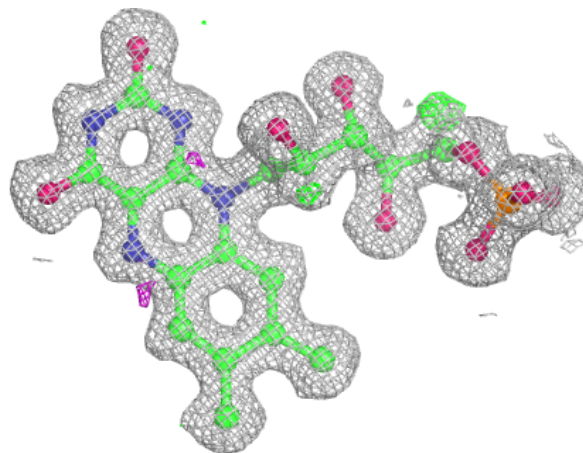
Electron density around W88 B 401 (A):

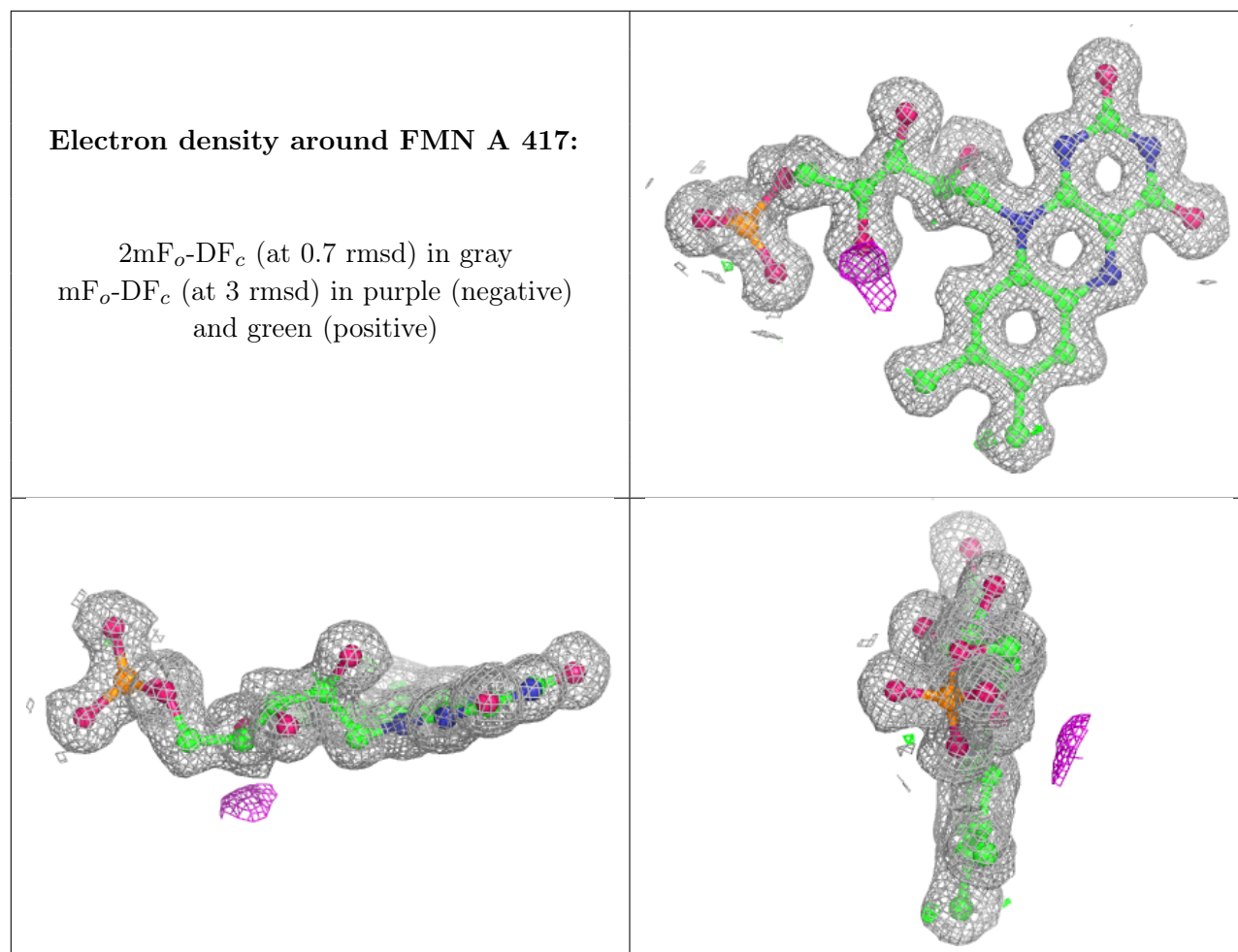
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around FMN B 415:

$2mF_o-DF_c$ (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.