WORLDWIDE wwPDB PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report (i)

Nov 3, 2024 – 03:27 am GMT

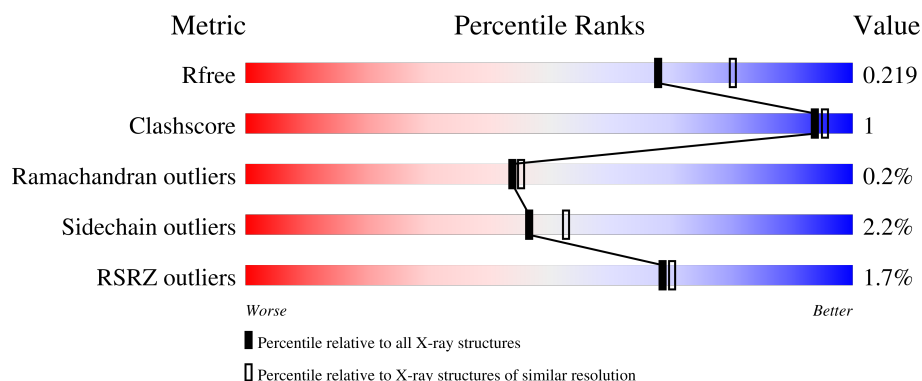|		
PDB ID	:	6GOS
Title	:	E. coli Microcin synthetase McbBCD complex with pro-MccB17 bound
Authors	:	Ghilarov, D.; Stevenson, C.E.M.; Travin, D.Y.; Piskunova, J.; Serebryakova, M.; Maxwell, A.; Lawson, D.M.; Severinov, K.
Deposited on	:	2018-06-04
Resolution	:	2.10 Å(reported)

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 2.10 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	Percentile Ranks	Value
Rfree		0.219
Clashscore		1
Ramachandran outliers		0.2%
Sidechain outliers		2.2%
RSRZ outliers		1.7%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	6234 (2.10-2.10)
Clashscore	180529	6893 (2.10-2.10)
Ramachandran outliers	177936	6839 (2.10-2.10)
Sidechain outliers	177891	6840 (2.10-2.10)
RSRZ outliers	164620	6234 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	68	10% — 34% 6% 60%
2	1	295	2% — 91% 5% ·
2	2	295	2% — 89% 6% ·
3	C	272	95% · ·
4	D	396	94% 6%

WORLDWIDE PDB
PROTEIN DATA BANK

2　Entry composition ⓘ

There are 11 unique types of molecules in this entry. The entry contains 10446 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 Bacteriocin microcin B17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	27	195	119	36	38	2	0	0	0

There are 23 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	MET	-	initiating methionine	UNP P05834
A	-6	GLY	-	expression tag	UNP P05834
A	-5	HIS	-	expression tag	UNP P05834
A	-4	HIS	-	expression tag	UNP P05834
A	-3	HIS	-	expression tag	UNP P05834
A	-2	HIS	-	expression tag	UNP P05834
A	-1	HIS	-	expression tag	UNP P05834
A	0	HIS	-	expression tag	UNP P05834
A	39	OTZ	GLY	modified residue	UNP P05834
A	39	OTZ	SER	modified residue	UNP P05834
A	39	OTZ	CYS	modified residue	UNP P05834
A	45	F75	GLY	modified residue	UNP P05834
A	45	F75	CYS	modified residue	UNP P05834
A	47	TOZ	GLY	modified residue	UNP P05834
A	47	TOZ	CYS	modified residue	UNP P05834
A	47	TOZ	SER	modified residue	UNP P05834
A	49	TOZ	GLY	modified residue	UNP P05834
A	49	TOZ	CYS	modified residue	UNP P05834
A	49	TOZ	SER	modified residue	UNP P05834
A	54	F6N	GLY	modified residue	UNP P05834
A	54	F6N	SER	modified residue	UNP P05834
A	56	F6N	GLY	modified residue	UNP P05834
A	56	F6N	SER	modified residue	UNP P05834

- Molecule 2 is a protein called Microcin B17-processing protein McbB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	1	284	Total 2329	C 1493	N 390	O 432	S 14	0	7	0
2	2	283	Total 2220	C 1423	N 368	O 418	S 11	0	1	0

- Molecule 3 is a protein called Microcin B17-processing protein McbC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	265	Total 2078	C 1334	N 351	O 385	S 8	0	0	0

- Molecule 4 is a protein called Microcin B17-processing protein McbD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	396	Total 3141	C 2007	N 514	O 602	S 18	0	1	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	171	ARG	THR	conflict	UNP P23186

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	1	1	Total 1	Zn 1	0	0
5	2	1	Total 1	Zn 1	0	0

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O_4S).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	1	1	Total 5	O 4	S 1	0	0

- Molecule 7 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	1	1	Total 1	Cl 1	0	0
7	D	1	Total 1	Cl 1	0	0

- Molecule 8 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).
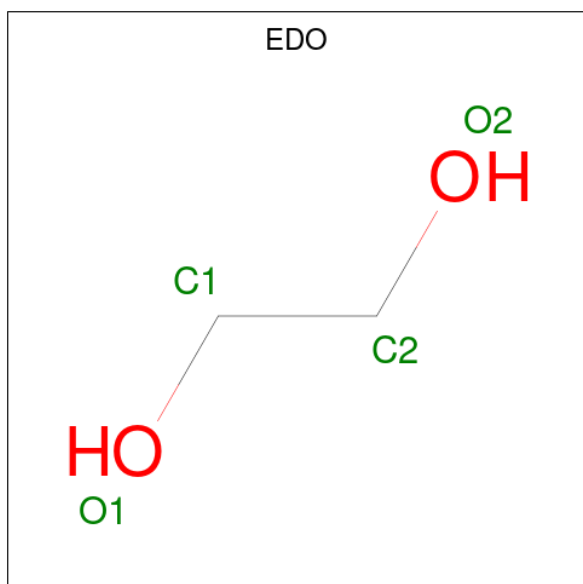
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	2	1	Total 4	C 2	O 2	0	0
8	2	1	Total 4	C 2	O 2	0	0
8	2	1	Total 8	C 4	O 4	0	1
8	D	1	Total 4	C 2	O 2	0	0
8	D	1	Total 4	C 2	O 2	0	0
8	D	1	Total 4	C 2	O 2	0	0

- Molecule 9 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: $C_{17}H_{21}N_4O_9P$).

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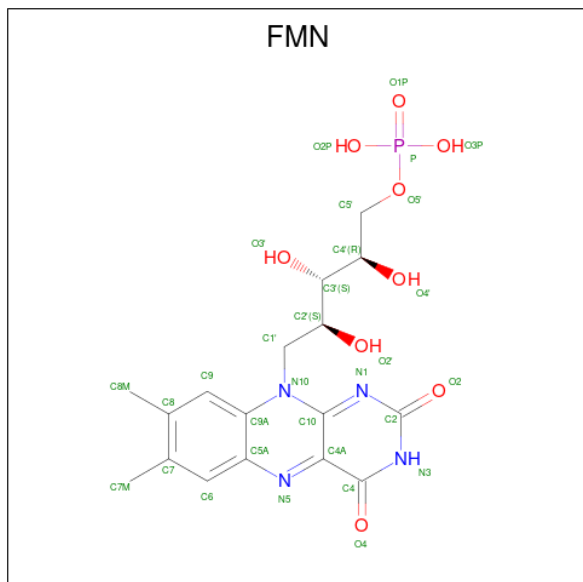
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	C	1	Total 31	C 17	N 4	O 9	P 1	0	0

- Molecule 10 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).

GOL

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

- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	6	Total 7	O 7	0	1
11	1	103	Total 108	O 108	0	5
11	2	83	Total 89	O 89	0	6
11	C	98	Total 102	O 102	0	4
11	D	95	Total 103	O 103	0	8

3   Residue-property plots ⓘ

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.
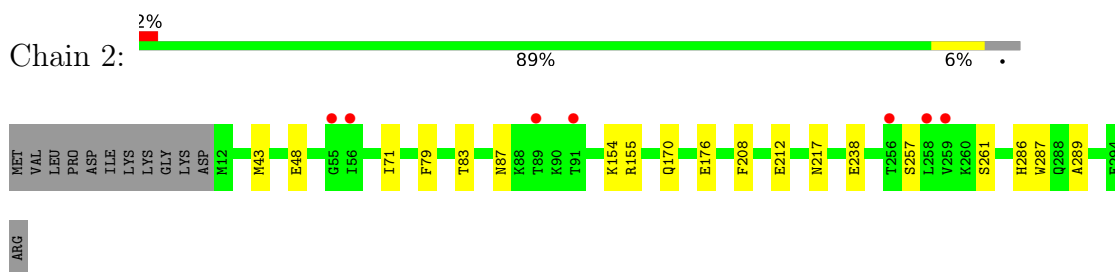
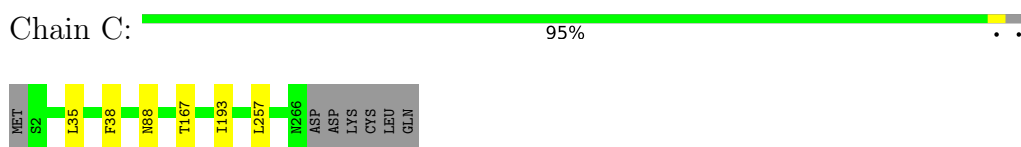• Molecule 1: Bacteriocin microcin B17
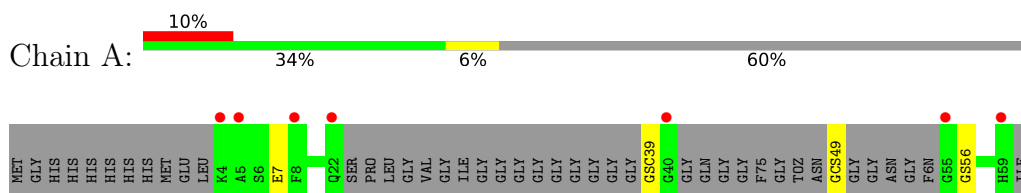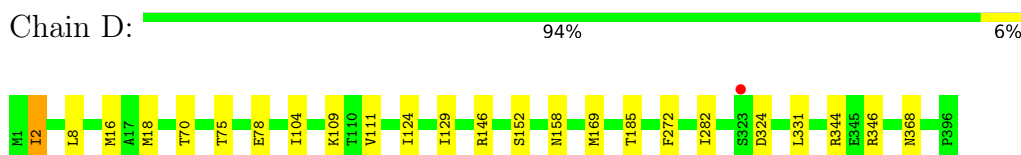

• Molecule 2: Microcin B17-processing protein McbB
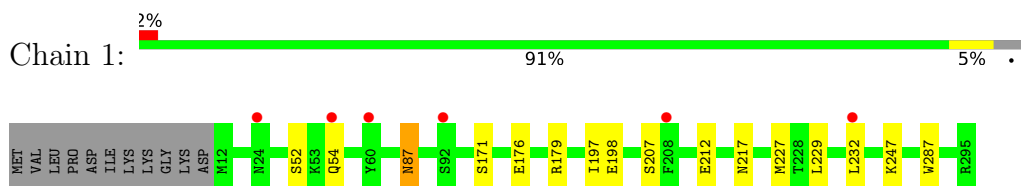
• Molecule 2: Microcin B17-processing protein McbB

• Molecule 3: Microcin B17-processing protein McbC

• Molecule 4: Microcin B17-processing protein McbD

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	180.96Å 83.40Å 86.90Å 90.00° 91.45° 90.00°	Depositor
Resolution (Å)	57.39 – 2.10 57.39 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.8 (57.39-2.10) 99.8 (57.39-2.10)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	1.57 (at 2.10Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.172 , 0.212 0.180 , 0.219	Depositor DCC
R_{free} test set	3821 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	36.2	Xtriage
Anisotropy	0.315	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 39.0	EDS
L-test for twinning [2]	$<|L|> = 0.49, <L^2> = 0.32$	Xtriage
Estimated twinning fraction	0.016 for -h,-k,l	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	10446	wwPDB-VP
Average B, all atoms (Å^2)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.70% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $<|L|>$, $<L^2>$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: FMN, SO4, TOZ, GOL, F6N, EDO, CL, OTZ, ZN

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	0.64	0/155	0.69	0/202
2	1	0.53	0/2379	0.71	0/3220
2	2	0.55	0/2269	0.72	0/3088
3	C	0.51	0/2131	0.71	0/2900
4	D	0.52	0/3211	0.69	0/4357
All	All	0.53	0/10145	0.70	0/13767

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	195	0	151	0	0
2	1	2329	0	2304	8	0
2	2	2220	0	2124	7	0
3	C	2078	0	2005	2	0
4	D	3141	0	3041	11	0
5	1	1	0	0	0	0
5	2	1	0	0	0	0
6	1	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	1	1	0	0	0	0
7	D	1	0	0	0	0
8	2	16	0	24	0	0
8	D	12	0	18	0	0
9	C	31	0	19	0	0
10	D	6	0	8	0	0
11	1	108	0	0	0	0
11	2	89	0	0	1	0
11	A	7	0	0	0	0
11	C	102	0	0	0	0
11	D	103	0	0	0	0
All	All	10446	0	9694	26	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 1.

The worst 5 of 26 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)
2:1:197:ILE:HD11	2:1:229:LEU:HD21	1.54	0.89
2:1:87:ASN:C	2:1:87:ASN:HD22	1.79	0.82
4:D:169:MET:CE	4:D:331:LEU:HD21	2.13	0.79
4:D:169:MET:HE1	4:D:331:LEU:HD21	1.78	0.64
4:D:169:MET:HE3	4:D:331:LEU:HD21	1.80	0.64

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	19/68 (28%)	19 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	1	289/295 (98%)	283 (98%)	4 (1%)	2 (1%)	19	16
2	2	282/295 (96%)	271 (96%)	11 (4%)	0	100	100
3	C	263/272 (97%)	258 (98%)	4 (2%)	1 (0%)	30	29
4	D	395/396 (100%)	388 (98%)	6 (2%)	1 (0%)	37	37
All	All	1248/1326 (94%)	1219 (98%)	25 (2%)	4 (0%)	44	37

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	1	54[A]	GLN
2	1	54[B]	GLN
3	C	88	ASN
4	D	2	ILE

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	15/37 (40%)	14 (93%)	1 (7%)	13	11
2	1	262/276 (95%)	258 (98%)	4 (2%)	60	67
2	2	242/276 (88%)	233 (96%)	9 (4%)	29	31
3	C	222/239 (93%)	221 (100%)	1 (0%)	86	91
4	D	341/351 (97%)	332 (97%)	9 (3%)	41	46
All	All	1082/1179 (92%)	1058 (98%)	24 (2%)	47	53

5 of 24 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	167	THR
4	D	146	ARG
4	D	16	MET
4	D	152	SER
2	2	87	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
2	1	14	ASN
2	1	87	ASN
2	1	97	ASN
2	1	217	ASN
2	2	286	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

3 non-standard protein/DNA/RNA residues 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	$\#|Z| > 2$
1	TOZ	A	49	-	10,15,16	0.64	0	3,20,22	4.08	1 (33%)
1	F6N	A	56	1	5,9,10	1.31	1 (20%)	1,11,13	5.69	1 (100%)
1	OTZ	A	39	1	10,15,16	1.37	2 (20%)	2,20,22	5.81	2 (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
1	TOZ	A	49	-	-	0/0/8/10	0/2/2/2
1	F6N	A	56	1	-	0/0/4/6	0/1/1/1
1	OTZ	A	39	1	-	0/0/8/10	0/2/2/2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	56	F6N	CA2-C	2.54	1.51	1.48
1	A	39	OTZ	CA2-C	2.52	1.51	1.48
1	A	39	OTZ	C4-N3	2.25	1.34	1.31

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	39	OTZ	O-C-CA2	-7.79	116.83	124.22
1	A	49	TOZ	O-C-CA2	-7.00	117.59	124.22
1	A	56	F6N	O-C-CA2	-5.69	118.83	124.22
1	A	39	OTZ	C3-C4-N3	2.60	131.16	124.47

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 14 ligands modelled in this entry, 4 are monoatomic - leaving 10 for Mogul analysis.

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	$\#|Z| > 2$
8	EDO	D	404	-	3,3,3	0.50	0	2,2,2	0.25	0
10	GOL	D	405	-	5,5,5	0.24	0	5,5,5	0.40	0
8	EDO	2	404[A]	-	3,3,3	0.47	0	2,2,2	0.09	0
8	EDO	D	401	-	3,3,3	0.49	0	2,2,2	0.18	0
6	SO4	1	302	-	4,4,4	0.36	0	6,6,6	0.19	0
9	FMN	C	501	-	33,33,33	1.57	5 (15%)	48,50,50	1.41	9 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
8	EDO	2	404[B]	-	3,3,3	0.40	0	2,2,2	0.39	0
8	EDO	D	403	-	3,3,3	0.41	0	2,2,2	0.29	0
8	EDO	2	402	-	3,3,3	0.46	0	2,2,2	0.26	0
8	EDO	2	403	-	3,3,3	0.42	0	2,2,2	0.52	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
8	EDO	D	404	-	-	0/1/1/1	-
10	GOL	D	405	-	-	0/4/4/4	-
8	EDO	2	404[A]	-	-	1/1/1/1	-
8	EDO	D	401	-	-	1/1/1/1	-
9	FMN	C	501	-	-	0/18/18/18	0/3/3/3
8	EDO	2	404[B]	-	-	1/1/1/1	-
8	EDO	D	403	-	-	0/1/1/1	-
8	EDO	2	402	-	-	0/1/1/1	-
8	EDO	2	403	-	-	0/1/1/1	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	C	501	FMN	C9A-C5A	5.83	1.50	1.41
9	C	501	FMN	C8-C7	3.15	1.48	1.40
9	C	501	FMN	C4A-N5	2.71	1.36	1.30
9	C	501	FMN	C10-N10	2.06	1.41	1.37
9	C	501	FMN	C4-N3	-2.04	1.35	1.38

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	C	501	FMN	O4-C4-C4A	-2.80	119.17	126.60
9	C	501	FMN	O2-C2-N1	-2.74	117.29	121.83
9	C	501	FMN	C4A-C10-N1	-2.71	118.45	124.73
9	C	501	FMN	C4-C4A-N5	2.70	122.08	118.23
9	C	501	FMN	C10-N1-C2	2.56	122.02	116.90

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	2	404[A]	EDO	O1-C1-C2-O2
8	2	404[B]	EDO	O1-C1-C2-O2
8	D	401	EDO	O1-C1-C2-O2

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand FMN C 501
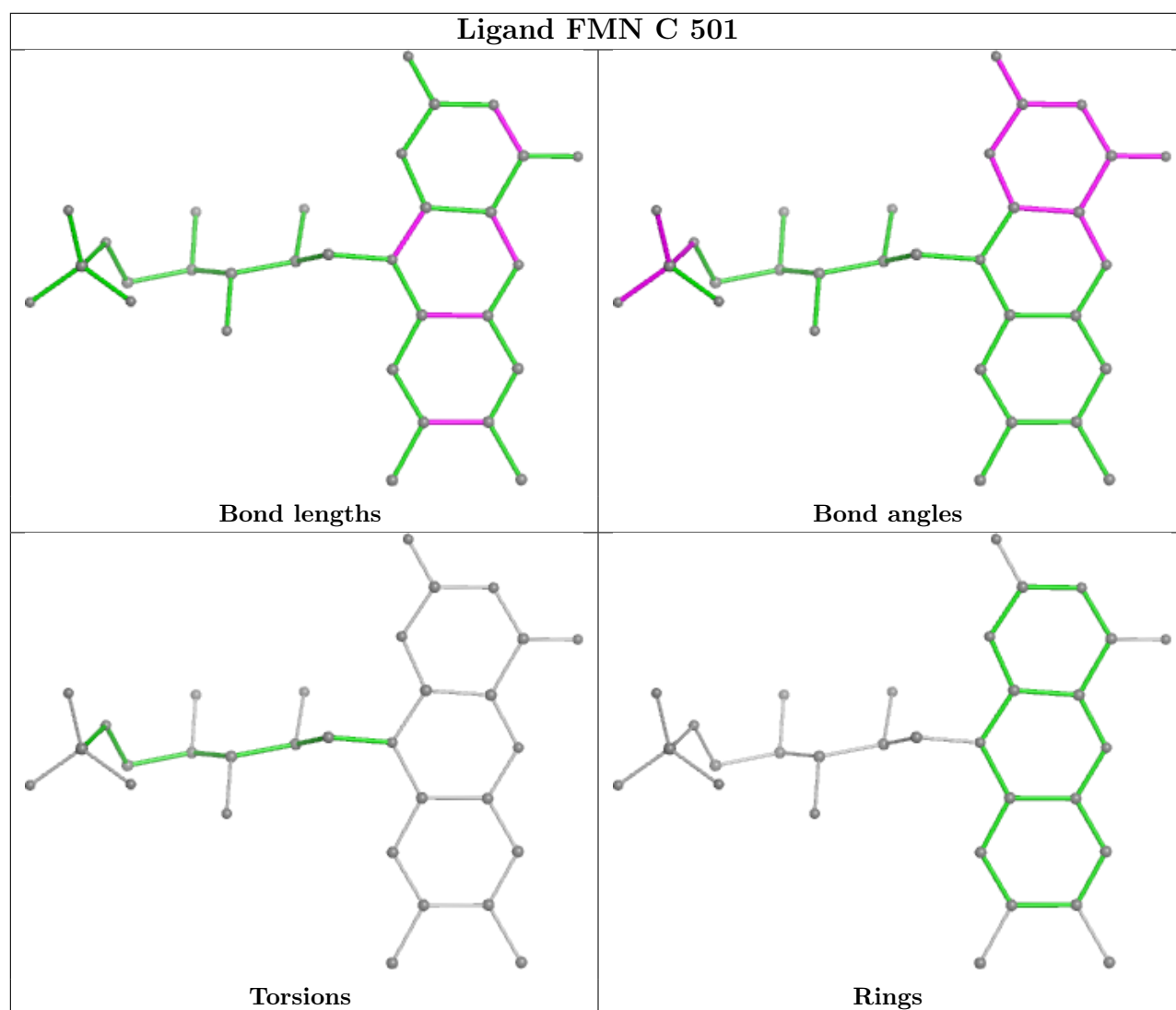
5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	24/68 (35%)	1.10	7 (29%)	1	1	42, 59, 82, 92	0
2	1	284/295 (96%)	-0.28	6 (2%)	63	65	14, 39, 64, 82	7 (2%)
2	2	283/295 (95%)	-0.11	7 (2%)	58	60	19, 43, 79, 105	1 (0%)
3	C	265/272 (97%)	-0.39	0	100	100	26, 41, 61, 76	0
4	D	396/396 (100%)	-0.18	1 (0%)	90	91	30, 47, 66, 79	1 (0%)
All	All	1252/1326 (94%)	-0.21	21 (1%)	69	70	14, 44, 70, 105	9 (0%)

The worst 5 of 21 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	2	258	LEU	4.5
1	A	40	GLY	3.9
2	1	54[A]	GLN	3.1
1	A	4	LYS	3.1
1	A	55	GLY	2.9

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

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.

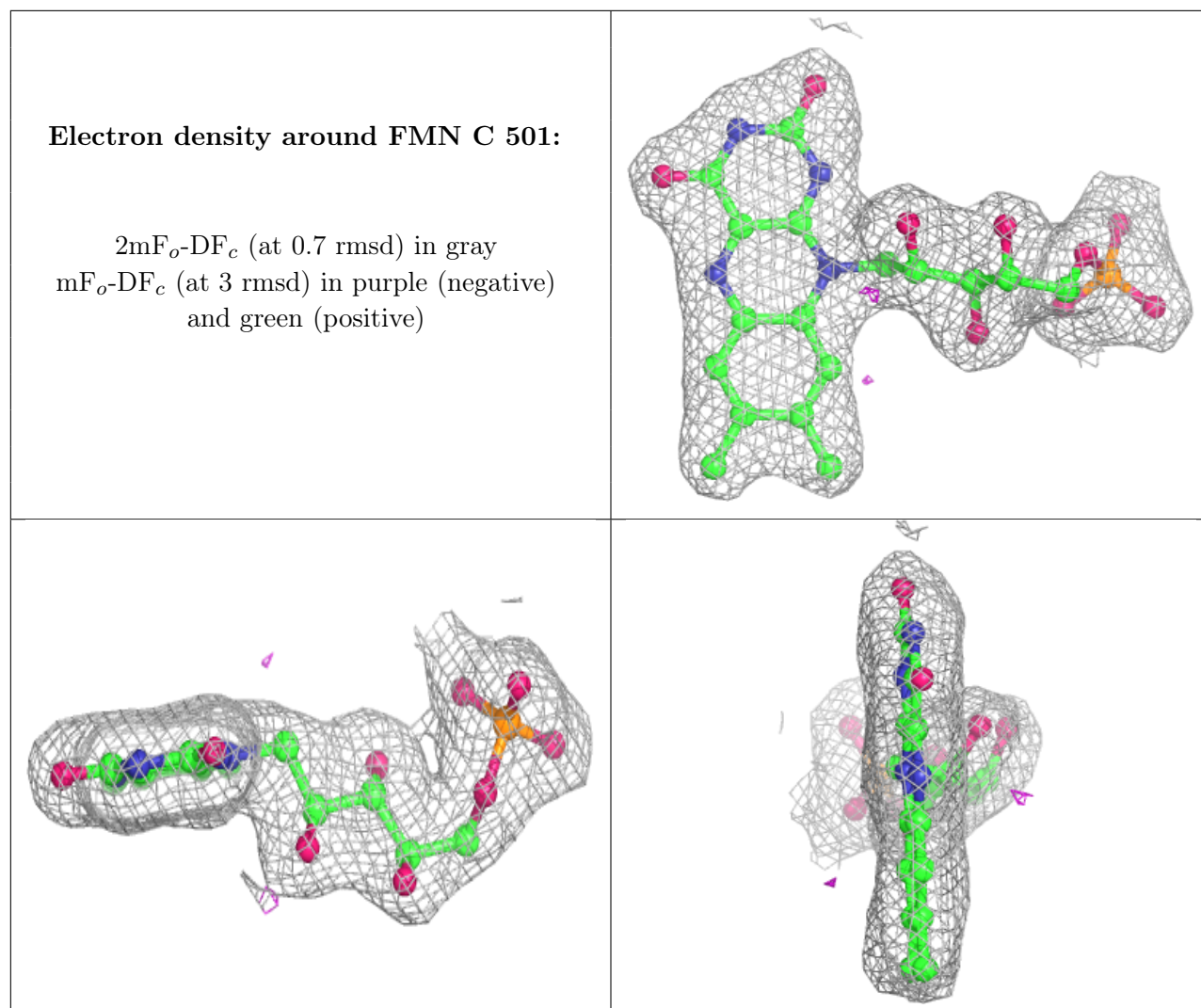| Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	TOZ	A	49	14/15	0.78	0.19	63,68,83,85	0
1	OTZ	A	39	14/15	0.83	0.14	69,73,88,90	0
1	F6N	A	56	9/10	0.95	0.12	57,60,63,64	0

6.3 Carbohydrates Ⓘ

There are no monosaccharides 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
8	EDO	D	404	4/4	0.85	0.13	59,60,68,69	0
8	EDO	D	403	4/4	0.87	0.18	53,55,57,58	0
8	EDO	2	404[A]	4/4	0.88	0.16	46,48,49,50	4
8	EDO	2	404[B]	4/4	0.88	0.16	35,36,38,38	4
8	EDO	2	403	4/4	0.90	0.13	58,59,61,61	0
6	SO4	1	302	5/5	0.91	0.09	62,65,76,78	0
7	CL	D	402	1/1	0.93	0.08	68,68,68,68	0
7	CL	1	303	1/1	0.93	0.15	58,58,58,58	0
10	GOL	D	405	6/6	0.93	0.08	44,53,57,68	0
8	EDO	D	401	4/4	0.95	0.07	42,44,45,49	0
8	EDO	2	402	4/4	0.95	0.09	41,48,49,53	0
9	FMN	C	501	31/31	0.97	0.05	31,35,40,40	0
5	ZN	2	401	1/1	0.99	0.02	33,33,33,33	0
5	ZN	1	301	1/1	1.00	0.01	31,31,31,31	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 FMN C 501:

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

6.5 Other polymers (i)

There are no such residues in this entry.