Full wwPDB X-ray Structure Validation Report ⓘ

Oct 26, 2024 – 02:25 PM EDT

PDB ID	:	6P3I
Title	:	The structure of condensation and adenylation domains of teixobactin-producing nonribosomal peptide synthetase Txo1 serine module in complex with Mg
Authors	:	Tan, K.; Zhou, M.; Jedrzejczak, R.; Babnigg, G.; Joachimiak, A.; Center for Structural Genomics of Infectious Diseases (CSGID)
Deposited on	:	2019-05-23
Resolution	:	2.15 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

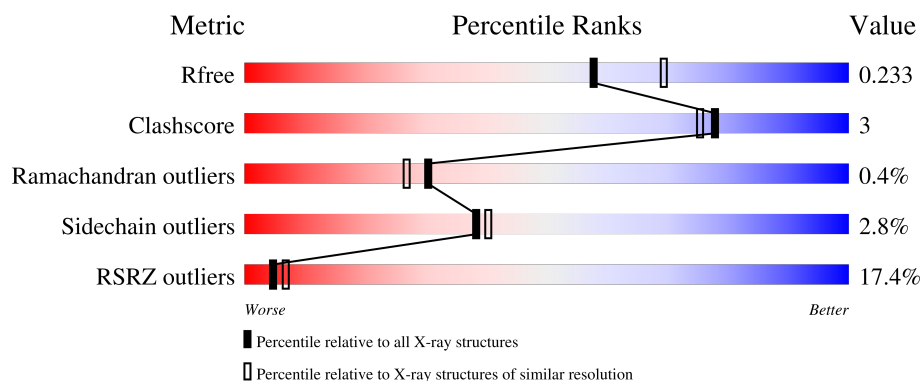|		
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

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 2.15 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		0.233
Clashscore		3
Ramachandran outliers		0.4%
Sidechain outliers		2.8%
RSRZ outliers		17.4%

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	1881 (2.16-2.16)
Clashscore	180529	2047 (2.16-2.16)
Ramachandran outliers	177936	2027 (2.16-2.16)
Sidechain outliers	177891	2026 (2.16-2.16)
RSRZ outliers	164620	1882 (2.16-2.16)

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	873	16% / 86% / 8% / 5%

2 Entry composition ⓘ

There are 5 unique types of molecules in this entry. The entry contains 6563 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 Txo1.

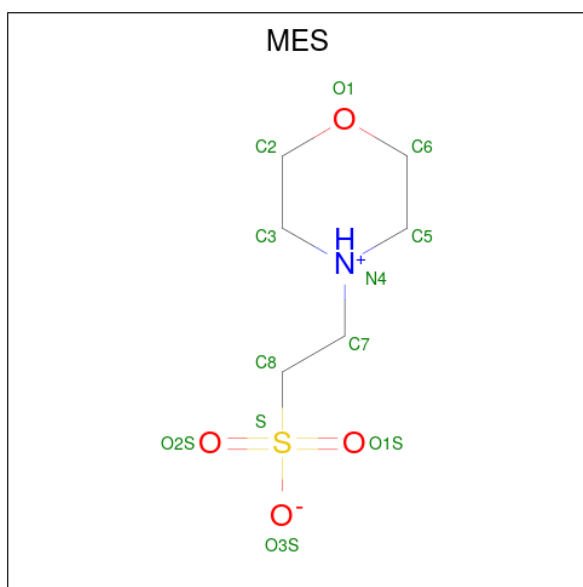| Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	830	Total	C	N	O	S	Se	0	4	0
			6329	3995	1160	1152	7	15			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2137	SER	-	expression tag	UNP A0A0B5GUD2
A	2138	ASN	-	expression tag	UNP A0A0B5GUD2
A	2139	ALA	-	expression tag	UNP A0A0B5GUD2

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		

- Molecule 3 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).

MES

O1

C2 C6

C3 H C5
N+
N4

C7

C8

S

O2S O S O O1S

O−

O3S

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
3	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
3	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O$_4$S).

SO4

O1

O

O3 O− S O− O4

S

O

O2

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

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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	117	Total 117	O 117	0	0

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: Txo1
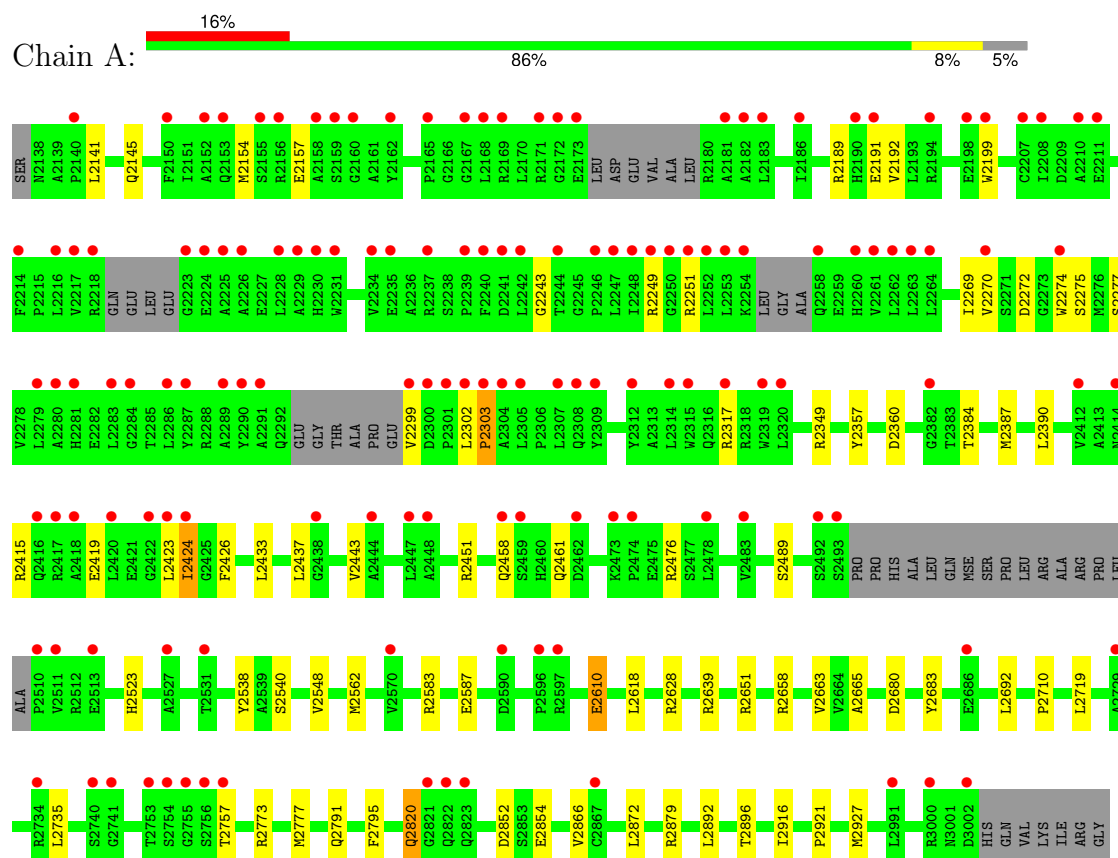
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	154.49Å 90.66Å 98.80Å 90.00° 106.00° 90.00°	Depositor
Resolution (Å)	45.33 – 2.15 45.33 – 2.15	Depositor EDS
% Data completeness (in resolution range)	98.5 (45.33-2.15) 91.0 (45.33-2.15)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.36 (at 2.14Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.201 , 0.231 0.205 , 0.233	Depositor DCC
R_{free} test set	3437 reflections (4.82%)	wwPDB-VP
Wilson B-factor (Å^2)	46.3	Xtriage
Anisotropy	0.404	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 56.3	EDS
L-test for twinning[2]	$< |L| > = 0.48$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	6563	wwPDB-VP
Average B, all atoms (Å^2)	86.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.08% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, MES, MG

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	0.23	0/6458	0.41	0/8779

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 (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	6329	0	6112	34	0
2	A	1	0	0	0	0
3	A	36	0	36	1	0
4	A	80	0	0	1	0
5	A	117	0	0	0	0
All	All	6563	0	6148	34	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 3.

All (34) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2390:LEU:HD11	1:A:2433:LEU:HD13	1.78	0.63
1:A:2249:ARG:HH21	1:A:2251:ARG:HE	1.47	0.61
1:A:2658:ARG:NH1	4:A:3118:SO4:O3	2.34	0.60
1:A:2773:ARG:HH12	1:A:2777:MSE:SE	2.36	0.58
1:A:2189:ARG:NH1	1:A:2303:PRO:O	2.36	0.57
1:A:2618:LEU:HD21	1:A:2663:VAL:HB	1.88	0.54
1:A:2665:ALA:HB2	1:A:2719:LEU:HD11	1.89	0.54
1:A:2189:ARG:NH1	1:A:2299:VAL:O	2.41	0.53
1:A:2384:THR:H	1:A:2387:MSE:SE	2.41	0.53
1:A:2896:THR:H	3:A:3103:MES:H72	1.75	0.51
1:A:2272:ASP:H	1:A:2275:SER:HB2	1.74	0.51
1:A:2415:ARG:NH2	1:A:2423:LEU:O	2.42	0.51
1:A:2458:GLN:O	1:A:2461:GLN:NE2	2.37	0.50
1:A:2269:ILE:HG23	1:A:2270:VAL:HG13	1.93	0.50
1:A:2489:SER:OG	1:A:2523:HIS:ND1	2.43	0.50
1:A:2639:ARG:HG2	1:A:2735:LEU:HD21	1.94	0.49
1:A:2387:MSE:HE1	1:A:2451:ARG:HG3	1.93	0.49
1:A:2538:TYR:CG	1:A:2548:VAL:HG21	2.47	0.49
1:A:2157:GLU:HG3	1:A:2357:TYR:CG	2.49	0.47
1:A:2852:ASP:OD1	1:A:2879:ARG:NH1	2.42	0.47
1:A:2610:GLU:OE1	1:A:2628[A]:ARG:NH2	2.46	0.47
1:A:2866:VAL:HG13	1:A:2892:LEU:HD13	1.97	0.47
1:A:2443:VAL:HG13	1:A:2562:MSE:HE2	1.96	0.46
1:A:2360:ASP:HB3	1:A:2538:TYR:CZ	2.51	0.46
1:A:2921:PRO:HB3	1:A:2927:MSE:HG2	1.97	0.46
1:A:2141:LEU:HD23	1:A:2145:GLN:HB3	1.98	0.44
1:A:2692:LEU:HD21	1:A:2710:PRO:HB3	2.00	0.43
1:A:2274:TRP:O	1:A:2277:SER:OG	2.24	0.43
1:A:2349:ARG:NH2	1:A:2540:SER:O	2.51	0.43
1:A:2872:LEU:HD23	1:A:2916:ILE:HG21	2.01	0.41
1:A:2583:ARG:HA	1:A:2587:GLU:HB2	2.03	0.41
1:A:2154:MSE:HA	1:A:2157:GLU:HB3	2.03	0.40
1:A:2275:SER:HB3	1:A:2424:ILE:HB	2.03	0.40
1:A:2680:ASP:HB3	1:A:2683:TYR:CD2	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	822/873 (94%)	801 (97%)	18 (2%)	3 (0%)	30　27

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2303	PRO
1	A	2820	GLN
1	A	2243	GLY

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	620/685 (90%)	603 (97%)	17 (3%)	40　42

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2191	GLU
1	A	2192	VAL
1	A	2199	TRP
1	A	2302	LEU
1	A	2317	ARG
1	A	2419	GLU
1	A	2424	ILE
1	A	2426	PHE

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Mol	Chain	Res	Type
1	A	2437	LEU
1	A	2476	ARG
1	A	2610	GLU
1	A	2651	ARG
1	A	2757	THR
1	A	2791	GLN
1	A	2795	PHE
1	A	2820	GLN
1	A	2854	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2745	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 20 ligands modelled in this entry, 1 is monoatomic - leaving 19 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
4	SO4	A	3112	-	4,4,4	0.24	0	6,6,6	0.07	0
3	MES	A	3104	-	12,12,12	2.35	1 (8%)	15,16,16	2.43	5 (33%)
4	SO4	A	3110	-	4,4,4	0.23	0	6,6,6	0.09	0
4	SO4	A	3119	-	4,4,4	0.24	0	6,6,6	0.07	0
4	SO4	A	3108	-	4,4,4	0.24	0	6,6,6	0.08	0
4	SO4	A	3105	-	4,4,4	0.23	0	6,6,6	0.08	0
4	SO4	A	3107	-	4,4,4	0.23	0	6,6,6	0.08	0
3	MES	A	3103	2	12,12,12	2.34	1 (8%)	15,16,16	1.92	4 (26%)
4	SO4	A	3117	-	4,4,4	0.23	0	6,6,6	0.08	0
3	MES	A	3102	-	12,12,12	2.31	1 (8%)	15,16,16	1.94	3 (20%)
4	SO4	A	3113	-	4,4,4	0.23	0	6,6,6	0.07	0
4	SO4	A	3109	-	4,4,4	0.24	0	6,6,6	0.07	0
4	SO4	A	3106	-	4,4,4	0.23	0	6,6,6	0.10	0
4	SO4	A	3111	-	4,4,4	0.23	0	6,6,6	0.07	0
4	SO4	A	3120	-	4,4,4	0.23	0	6,6,6	0.07	0
4	SO4	A	3115	-	4,4,4	0.23	0	6,6,6	0.08	0
4	SO4	A	3116	-	4,4,4	0.23	0	6,6,6	0.07	0
4	SO4	A	3118	-	4,4,4	0.24	0	6,6,6	0.08	0
4	SO4	A	3114	-	4,4,4	0.23	0	6,6,6	0.07	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	MES	A	3103	2	-	5/6/14/14	0/1/1/1
3	MES	A	3102	-	-	5/6/14/14	0/1/1/1
3	MES	A	3104	-	-	1/6/14/14	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	3104	MES	C8-S	-7.88	1.66	1.77
3	A	3103	MES	C8-S	-7.82	1.66	1.77
3	A	3102	MES	C8-S	-7.74	1.66	1.77

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	3104	MES	C5-N4-C3	5.37	120.40	108.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	3102	MES	C5-N4-C3	4.79	119.16	108.84
3	A	3104	MES	C6-C5-N4	-4.08	103.92	110.12
3	A	3103	MES	C5-N4-C3	3.67	116.76	108.84
3	A	3103	MES	C6-C5-N4	-3.63	104.60	110.12
3	A	3104	MES	C7-N4-C5	3.57	120.74	111.24
3	A	3104	MES	C7-N4-C3	2.80	118.69	111.24
3	A	3103	MES	C7-N4-C5	2.71	118.47	111.24
3	A	3102	MES	C7-N4-C5	2.23	117.18	111.24
3	A	3104	MES	O2S-S-C8	2.20	110.06	106.73
3	A	3103	MES	O2S-S-C8	2.14	109.97	106.73
3	A	3102	MES	C7-N4-C3	2.10	116.84	111.24

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	3102	MES	C7-C8-S-O1S
3	A	3102	MES	C7-C8-S-O2S
3	A	3103	MES	C8-C7-N4-C5
3	A	3104	MES	C8-C7-N4-C5
3	A	3103	MES	C7-C8-S-O3S
3	A	3102	MES	C7-C8-S-O3S
3	A	3102	MES	C8-C7-N4-C5
3	A	3103	MES	C7-C8-S-O1S
3	A	3103	MES	C7-C8-S-O2S
3	A	3103	MES	N4-C7-C8-S
3	A	3102	MES	C8-C7-N4-C3

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	3103	MES	1	0
4	A	3118	SO4	1	0

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(Å²)	Q<0.9
1	A	816/873 (93%)	0.90	142 (17%)	5	7	28, 72, 170, 208	3 (0%)

All (142) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	2286	LEU	7.9
1	A	2248	ILE	6.8
1	A	2307	LEU	6.6
1	A	2247	LEU	6.2
1	A	2253	LEU	5.7
1	A	2216	LEU	5.5
1	A	2290	TYR	5.3
1	A	2424	ILE	5.2
1	A	2252	LEU	5.0
1	A	2493	SER	5.0
1	A	2492	SER	4.8
1	A	2158	ALA	4.6
1	A	2152	ALA	4.6
1	A	2301	PRO	4.6
1	A	2302	LEU	4.4
1	A	2300	ASP	4.4
1	A	2153	GLN	4.4
1	A	2237	ARG	4.3
1	A	2168	LEU	4.3
1	A	2303	PRO	4.2
1	A	2217	VAL	4.2
1	A	2299	VAL	4.1
1	A	2305	LEU	4.1
1	A	2182	ALA	4.0
1	A	2181	ALA	4.0
1	A	2258	GLN	4.0
1	A	2234	VAL	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	3002	ASP	3.9
1	A	2319	TRP	3.9
1	A	2250	GLY	3.9
1	A	2231	TRP	3.8
1	A	2423	LEU	3.8
1	A	2284	GLY	3.8
1	A	2228	LEU	3.8
1	A	2262	LEU	3.8
1	A	2210	ALA	3.7
1	A	2270	VAL	3.7
1	A	2417	ARG	3.7
1	A	2308	GLN	3.6
1	A	2823	GLN	3.6
1	A	2821	GLY	3.6
1	A	2511	VAL	3.5
1	A	2160	GLY	3.5
1	A	2422	GLY	3.5
1	A	2753	THR	3.5
1	A	2740	SER	3.5
1	A	2183	LEU	3.5
1	A	2279	LEU	3.5
1	A	2312	TYR	3.4
1	A	2211	GLU	3.4
1	A	2186	ILE	3.4
1	A	2309	TYR	3.4
1	A	2246	PRO	3.3
1	A	2755	GLY	3.3
1	A	2274	TRP	3.3
1	A	2229	ALA	3.3
1	A	2199	TRP	3.3
1	A	2214	PHE	3.3
1	A	2218	ARG	3.3
1	A	2242	LEU	3.3
1	A	2459	SER	3.3
1	A	2171	ARG	3.2
1	A	2734[A]	ARG	3.2
1	A	2741	GLY	3.2
1	A	2462	ASP	3.1
1	A	2416	GLN	3.1
1	A	2173	GLU	3.1
1	A	2418	ALA	3.1
1	A	2444	ALA	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	2412	VAL	3.1
1	A	2420	LEU	3.0
1	A	2382	GLY	3.0
1	A	2414	ASN	2.9
1	A	2263	LEU	2.9
1	A	2261	VAL	2.9
1	A	2159	SER	2.9
1	A	2244	THR	2.9
1	A	2224	GLU	2.8
1	A	2254	LYS	2.8
1	A	2510	PRO	2.8
1	A	2289	ALA	2.8
1	A	2207	CYS	2.8
1	A	2991	LEU	2.8
1	A	2597	ARG	2.8
1	A	2287	TYR	2.8
1	A	2527	ALA	2.7
1	A	2169	ARG	2.7
1	A	2225	ALA	2.7
1	A	2729	ALA	2.7
1	A	2478	LEU	2.7
1	A	2754	SER	2.6
1	A	2756	SER	2.6
1	A	2447	LEU	2.6
1	A	2260	HIS	2.6
1	A	2241	ASP	2.6
1	A	2165	PRO	2.6
1	A	2239	PRO	2.6
1	A	2249	ARG	2.6
1	A	2226	ALA	2.6
1	A	2291	ALA	2.6
1	A	2483	VAL	2.6
1	A	2757	THR	2.6
1	A	2458	GLN	2.6
1	A	2283	LEU	2.6
1	A	2223	GLY	2.5
1	A	2280	ALA	2.5
1	A	2230	HIS	2.5
1	A	2448	ALA	2.5
1	A	2474	PRO	2.5
1	A	2251	ARG	2.5
1	A	2150	PHE	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	2438	GLY	2.5
1	A	2590	ASP	2.5
1	A	2314	LEU	2.4
1	A	2596	PRO	2.4
1	A	2686	GLU	2.4
1	A	2155	SER	2.4
1	A	2235	GLU	2.4
1	A	2190	HIS	2.4
1	A	2281	HIS	2.3
1	A	2304	ALA	2.3
1	A	2317	ARG	2.3
1	A	2570	VAL	2.3
1	A	2208	ILE	2.3
1	A	2264	LEU	2.3
1	A	2320	LEU	2.3
1	A	2162	TYR	2.3
1	A	2822	GLN	2.2
1	A	2191	GLU	2.2
1	A	2140	PRO	2.2
1	A	2172	GLY	2.2
1	A	2315	TRP	2.2
1	A	2473	LYS	2.1
1	A	2194	ARG	2.1
1	A	2531	THR	2.1
1	A	3000	ARG	2.1
1	A	2240	PHE	2.1
1	A	2198	GLU	2.1
1	A	2867	CYS	2.1
1	A	2156	ARG	2.1
1	A	2167	GLY	2.0
1	A	2513	GLU	2.0

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

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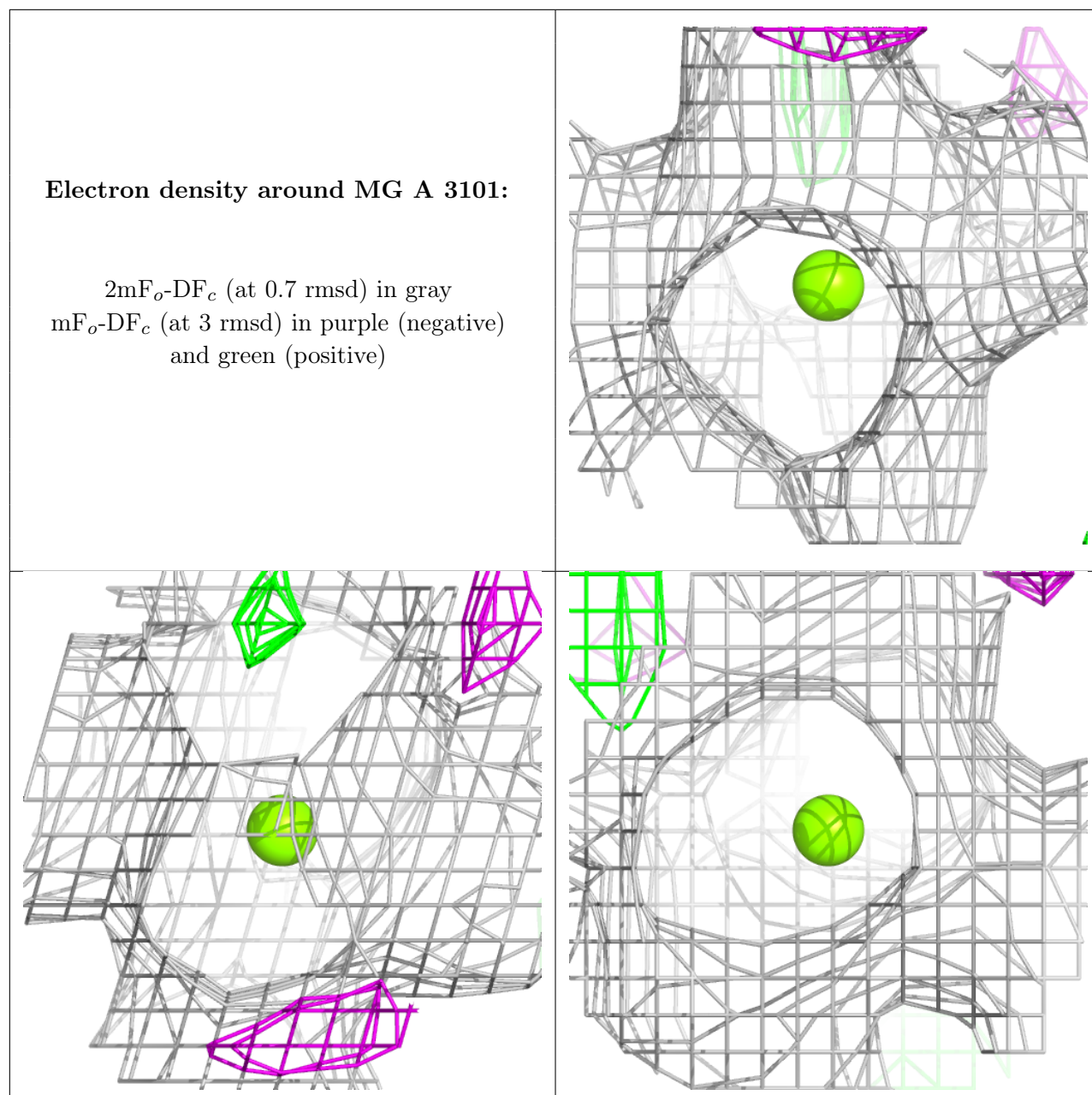
6.3 Carbohydrates ⓘ

There are no 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
4	SO4	A	3116	5/5	0.54	0.15	153,156,158,159	0
4	SO4	A	3118	5/5	0.55	0.22	160,164,165,167	0
4	SO4	A	3111	5/5	0.61	0.10	120,121,122,124	5
4	SO4	A	3120	5/5	0.67	0.11	163,164,165,167	0
3	MES	A	3104	12/12	0.68	0.24	139,146,196,206	0
4	SO4	A	3119	5/5	0.69	0.16	155,158,160,161	0
3	MES	A	3103	12/12	0.70	0.26	119,130,132,144	0
4	SO4	A	3110	5/5	0.71	0.12	122,122,124,129	5
4	SO4	A	3107	5/5	0.71	0.14	130,133,134,136	0
4	SO4	A	3115	5/5	0.72	0.15	166,167,168,169	5
4	SO4	A	3108	5/5	0.75	0.12	154,154,158,159	5
4	SO4	A	3114	5/5	0.81	0.19	161,162,162,162	5
4	SO4	A	3113	5/5	0.82	0.23	151,152,152,153	5
4	SO4	A	3106	5/5	0.83	0.11	91,102,104,105	5
4	SO4	A	3112	5/5	0.83	0.10	100,104,105,110	5
4	SO4	A	3117	5/5	0.83	0.25	146,149,152,152	5
4	SO4	A	3109	5/5	0.84	0.10	149,151,152,155	0
4	SO4	A	3105	5/5	0.88	0.10	130,132,133,134	0
3	MES	A	3102	12/12	0.92	0.12	73,84,97,98	0
2	MG	A	3101	1/1	0.99	0.04	50,50,50,50	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 MG A 3101:

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

6.5 Other polymers ⓘ

There are no such residues in this entry.