



Full wwPDB X-ray Structure Validation Report ⓘ

May 18, 2020 – 03:01 pm BST

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 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 : 2.11
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)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

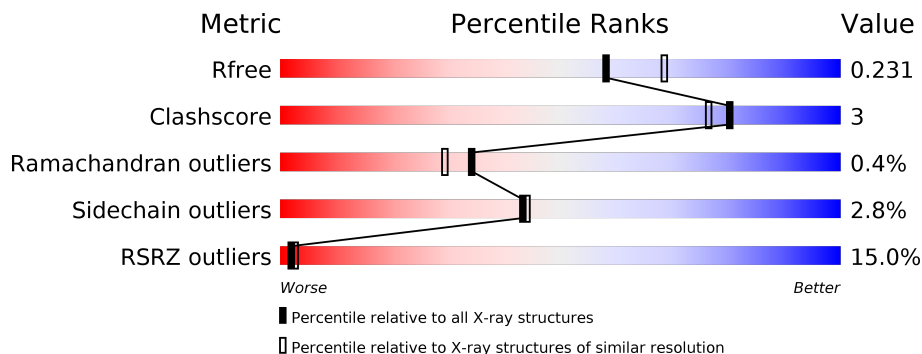
1 Overall quality at a glance

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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1479 (2.16-2.16)
Clashscore	141614	1585 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)
RSRZ outliers	127900	1456 (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 on 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	873	

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
			Total	C	N	O	S	Se			
1	A	830	6329	3995	1160	1152	7	15	0	4	0

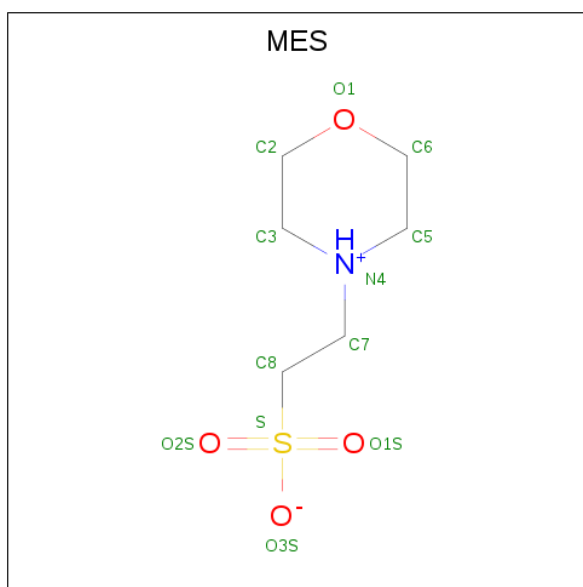
There are 3 discrepancies between the modelled and reference sequences:

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 author).

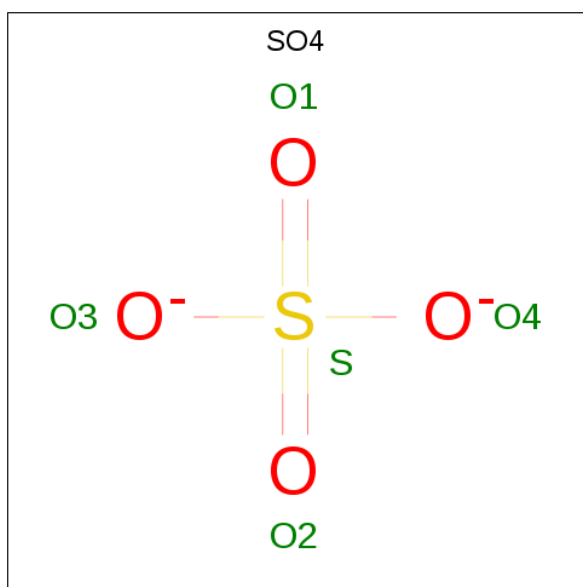
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		

- Molecule 3 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: C₆H₁₃NO₄S).



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

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

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

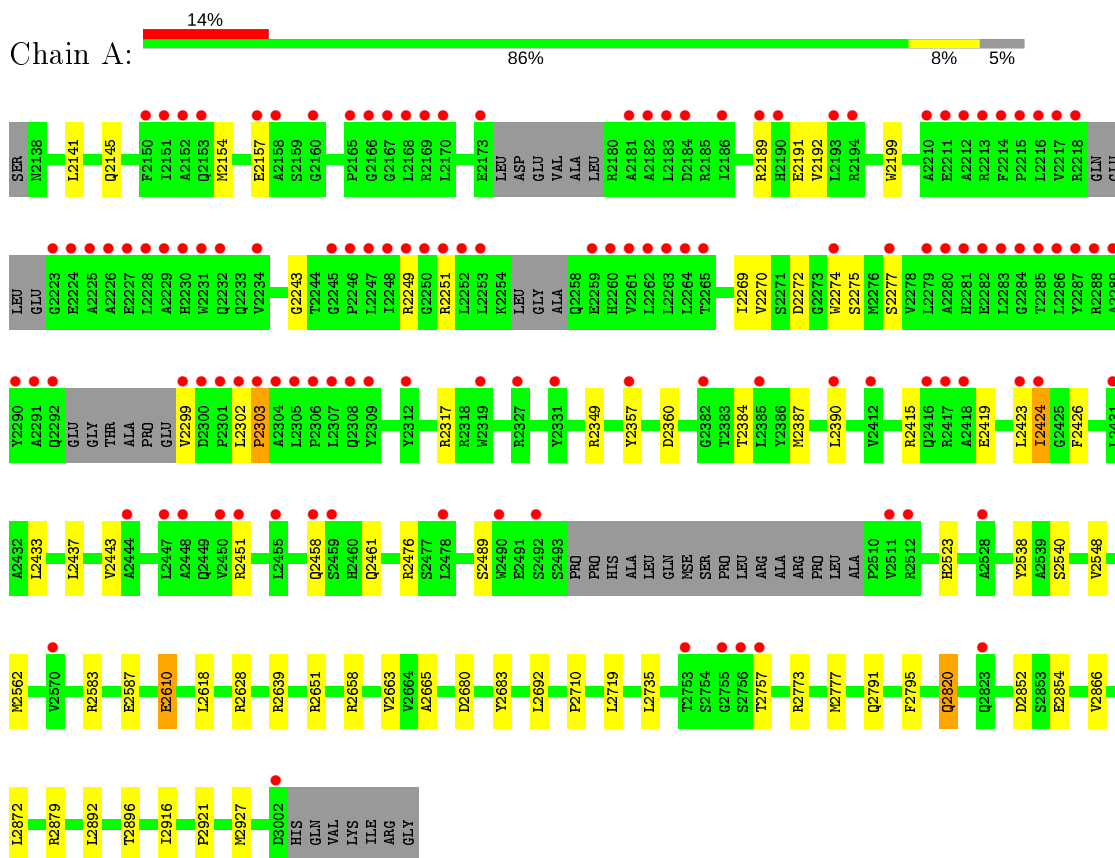
- Molecule 5 is water.

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

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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 47.49 – 2.14	Depositor EDS
% Data completeness (in resolution range)	98.5 (45.33-2.15) 90.6 (47.49-2.14)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.36 (at 2.14Å)	Xtrriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.201 , 0.231 0.201 , 0.231	Depositor DCC
R_{free} test set	3391 reflections (4.81%)	wwPDB-VP
Wilson B-factor (Å ²)	46.3	Xtrriage
Anisotropy	0.404	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 61.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
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

Xtrriage'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.*

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: MG, SO4, MES

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 [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	822/873 (94%)	801 (97%)	18 (2%)	3 (0%)	34 29

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 [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	620/685 (90%)	603 (97%)	17 (3%)	44 46

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

Some 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 [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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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
3	MES	A	3103	2	12,12,12	2.29	1 (8%)	14,16,16	2.04	5 (35%)
4	SO4	A	3106	-	4,4,4	0.14	0	6,6,6	0.07	0
4	SO4	A	3108	-	4,4,4	0.14	0	6,6,6	0.05	0
4	SO4	A	3110	-	4,4,4	0.14	0	6,6,6	0.08	0
3	MES	A	3104	-	12,12,12	2.30	1 (8%)	14,16,16	2.54	7 (50%)
4	SO4	A	3119	-	4,4,4	0.14	0	6,6,6	0.04	0
4	SO4	A	3107	-	4,4,4	0.14	0	6,6,6	0.05	0
4	SO4	A	3113	-	4,4,4	0.14	0	6,6,6	0.05	0
4	SO4	A	3109	-	4,4,4	0.14	0	6,6,6	0.04	0
4	SO4	A	3111	-	4,4,4	0.14	0	6,6,6	0.05	0
4	SO4	A	3116	-	4,4,4	0.14	0	6,6,6	0.05	0
4	SO4	A	3115	-	4,4,4	0.14	0	6,6,6	0.05	0
3	MES	A	3102	-	12,12,12	2.26	1 (8%)	14,16,16	2.01	6 (42%)
4	SO4	A	3112	-	4,4,4	0.14	0	6,6,6	0.05	0
4	SO4	A	3117	-	4,4,4	0.14	0	6,6,6	0.05	0
4	SO4	A	3105	-	4,4,4	0.14	0	6,6,6	0.05	0
4	SO4	A	3114	-	4,4,4	0.14	0	6,6,6	0.05	0
4	SO4	A	3118	-	4,4,4	0.14	0	6,6,6	0.05	0
4	SO4	A	3120	-	4,4,4	0.14	0	6,6,6	0.05	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	3104	-	-	1/6/14/14	0/1/1/1
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

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	3104	MES	C8-S	-7.71	1.66	1.77
3	A	3103	MES	C8-S	-7.66	1.66	1.77
3	A	3102	MES	C8-S	-7.58	1.66	1.77

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	3104	MES	C5-N4-C3	5.14	120.40	108.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	3102	MES	C5-N4-C3	4.59	119.16	108.83
3	A	3104	MES	C6-C5-N4	-4.08	103.92	110.10
3	A	3104	MES	C7-N4-C5	3.72	120.74	111.23
3	A	3103	MES	C6-C5-N4	-3.63	104.60	110.10
3	A	3103	MES	C5-N4-C3	3.52	116.76	108.83
3	A	3104	MES	C7-N4-C3	2.92	118.69	111.23
3	A	3103	MES	C7-N4-C5	2.83	118.47	111.23
3	A	3104	MES	O2S-S-C8	2.61	110.06	106.92
3	A	3103	MES	O2S-S-C8	2.53	109.97	106.92
3	A	3103	MES	O3S-S-C8	2.38	109.62	105.77
3	A	3102	MES	C7-N4-C5	2.32	117.18	111.23
3	A	3102	MES	O1S-S-C8	2.27	109.65	106.92
3	A	3102	MES	O3S-S-C8	2.23	109.38	105.77
3	A	3102	MES	C7-N4-C3	2.19	116.84	111.23
3	A	3104	MES	O1S-S-C8	2.15	109.51	106.92
3	A	3102	MES	O2S-S-C8	2.13	109.48	106.92
3	A	3104	MES	O3S-S-C8	2.03	109.06	105.77

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	3103	MES	C8-C7-N4-C5
3	A	3103	MES	N4-C7-C8-S
3	A	3104	MES	C8-C7-N4-C5
3	A	3102	MES	C7-C8-S-O1S
3	A	3102	MES	C7-C8-S-O2S
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	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(Å ²)	Q<0.9
1	A	816/873 (93%)	1.01	122 (14%) 2 3	42, 72, 170, 208	0

All (122) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	2252	LEU	19.4
1	A	2250	GLY	12.5
1	A	2262	LEU	11.8
1	A	2217	VAL	11.4
1	A	2216	LEU	10.9
1	A	2228	LEU	10.3
1	A	2247	LEU	10.3
1	A	2261	VAL	10.0
1	A	2218	ARG	9.9
1	A	2253	LEU	9.6
1	A	2225	ALA	9.2
1	A	2289	ALA	9.2
1	A	2305	LEU	9.1
1	A	2757	THR	8.9
1	A	2263	LEU	8.1
1	A	2226	ALA	8.0
1	A	2248	ILE	7.9
1	A	2756	SER	7.8
1	A	2284	GLY	7.8
1	A	2229	ALA	7.5
1	A	2251	ARG	7.2
1	A	2173	GLU	7.2
1	A	2190	HIS	7.2
1	A	2167	GLY	7.1
1	A	2231	TRP	6.9
1	A	2213	ARG	6.8
1	A	2183	LEU	6.7

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Mol	Chain	Res	Type	RSRZ
1	A	2279	LEU	6.6
1	A	2286	LEU	6.6
1	A	2215	PRO	6.6
1	A	2260	HIS	6.6
1	A	2214	PHE	6.2
1	A	2223	GLY	6.0
1	A	2212	ALA	5.9
1	A	2224	GLU	5.8
1	A	2511	VAL	5.8
1	A	2169	ARG	5.8
1	A	2234	VAL	5.7
1	A	2246	PRO	5.7
1	A	2280	ALA	5.5
1	A	2170	LEU	5.5
1	A	2249	ARG	5.5
1	A	2299	VAL	5.4
1	A	2227	GLU	5.4
1	A	2301	PRO	5.3
1	A	2186	ILE	5.3
1	A	2168	LEU	5.2
1	A	2291	ALA	5.1
1	A	2285	THR	5.0
1	A	2211	GLU	5.0
1	A	2309	TYR	5.0
1	A	2287	TYR	4.9
1	A	2290	TYR	4.8
1	A	2424	ILE	4.8
1	A	2283	LEU	4.7
1	A	2182	ALA	4.6
1	A	2448	ALA	4.6
1	A	2152	ALA	4.6
1	A	2308	GLN	4.5
1	A	2288	ARG	4.4
1	A	2418	ALA	4.4
1	A	2528	ALA	4.4
1	A	2416	GLN	4.3
1	A	2158	ALA	4.3
1	A	2264	LEU	4.3
1	A	2302	LEU	4.3
1	A	2382	GLY	4.3
1	A	2307	LEU	4.2
1	A	2300	ASP	4.2

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Mol	Chain	Res	Type	RSRZ
1	A	2292	GLN	4.1
1	A	2194	ARG	3.9
1	A	2447	LEU	3.9
1	A	2303	PRO	3.7
1	A	2455	LEU	3.7
1	A	2319	TRP	3.6
1	A	2210	ALA	3.5
1	A	2166	GLY	3.4
1	A	2450	VAL	3.3
1	A	2492	SER	3.3
1	A	2304	ALA	3.3
1	A	2245	GLY	3.3
1	A	2444	ALA	3.2
1	A	2417	ARG	3.2
1	A	2193	LEU	3.1
1	A	2281	HIS	3.1
1	A	2385	LEU	3.1
1	A	2412	VAL	3.0
1	A	2490	TRP	3.0
1	A	2512	ARG	3.0
1	A	2265	THR	2.9
1	A	2181	ALA	2.9
1	A	2306	PRO	2.9
1	A	2274	TRP	2.9
1	A	2282	GLU	2.8
1	A	2423	LEU	2.8
1	A	2153	GLN	2.7
1	A	2184	ASP	2.7
1	A	2151	ILE	2.7
1	A	2823	GLN	2.7
1	A	2312	TYR	2.7
1	A	2277	SER	2.7
1	A	2753	THR	2.7
1	A	2755	GLY	2.6
1	A	2327	ARG	2.5
1	A	2570	VAL	2.5
1	A	2478	LEU	2.4
1	A	2165	PRO	2.4
1	A	2157	GLU	2.4
1	A	2189	ARG	2.4
1	A	2331	TYR	2.3
1	A	2232	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	2451	ARG	2.3
1	A	2390	LEU	2.3
1	A	2259	GLU	2.3
1	A	2458	GLN	2.3
1	A	2150	PHE	2.2
1	A	2431	LEU	2.2
1	A	2160	GLY	2.1
1	A	2230	HIS	2.1
1	A	3002	ASP	2.1
1	A	2357	TYR	2.0
1	A	2459	SER	2.0

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 carbohydrates 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.

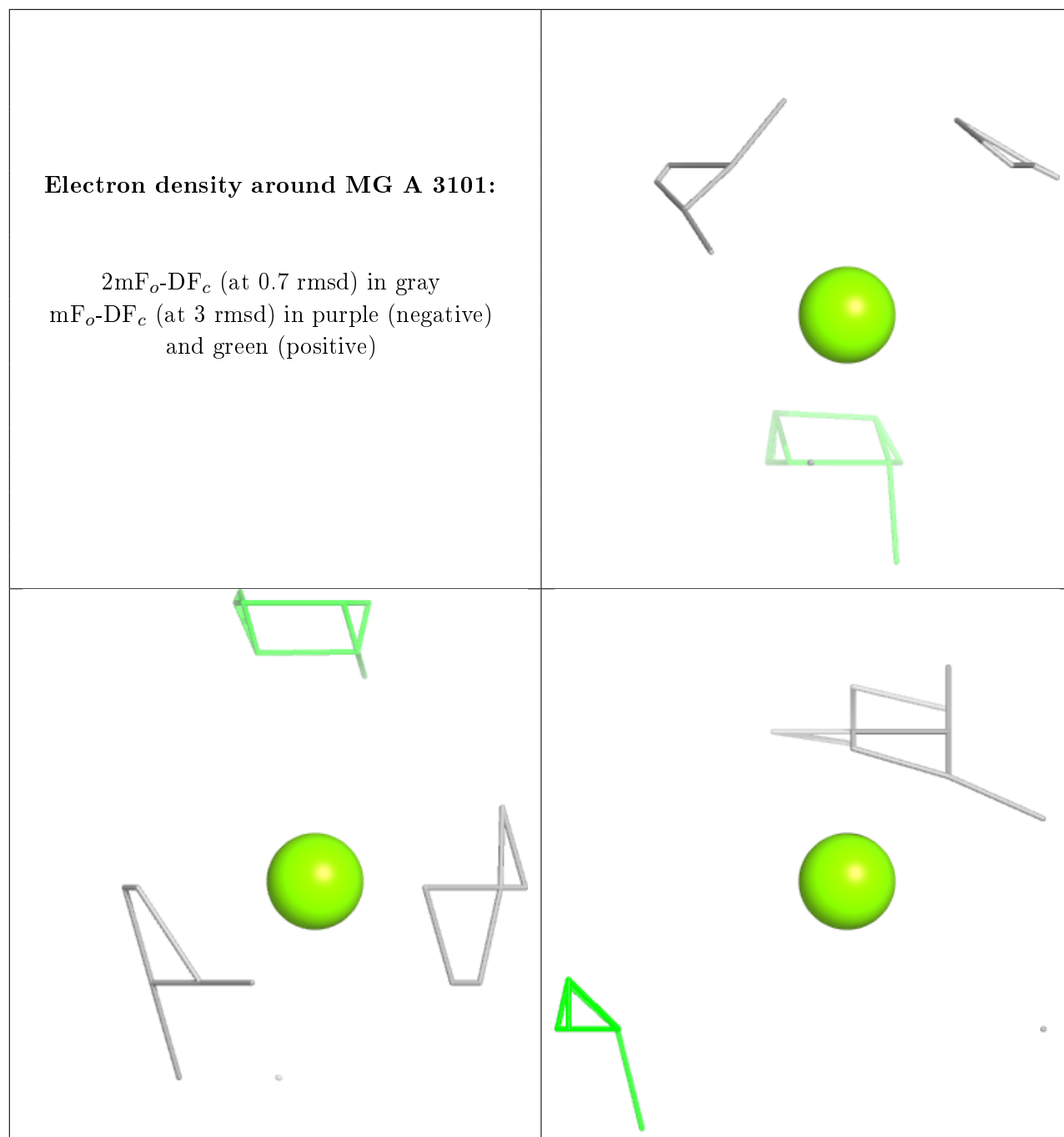
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	SO4	A	3115	5/5	0.65	0.27	166,167,168,169	5
3	MES	A	3104	12/12	0.68	0.34	139,146,196,206	0
4	SO4	A	3117	5/5	0.70	0.28	146,149,152,152	5
4	SO4	A	3116	5/5	0.73	0.22	153,156,158,159	0
4	SO4	A	3118	5/5	0.76	0.26	160,164,165,167	0
4	SO4	A	3119	5/5	0.77	0.23	155,158,160,161	0
4	SO4	A	3110	5/5	0.77	0.18	122,122,124,129	5
4	SO4	A	3113	5/5	0.79	0.22	151,152,152,153	5
3	MES	A	3103	12/12	0.80	0.28	119,130,132,144	0
4	SO4	A	3120	5/5	0.84	0.16	163,164,165,167	0
4	SO4	A	3106	5/5	0.84	0.17	91,102,104,105	5
4	SO4	A	3114	5/5	0.85	0.26	161,162,162,162	5

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	SO4	A	3109	5/5	0.87	0.15	149,151,152,155	0
4	SO4	A	3107	5/5	0.88	0.20	130,133,134,136	0
4	SO4	A	3112	5/5	0.88	0.31	100,104,105,110	5
4	SO4	A	3108	5/5	0.92	0.17	154,154,158,159	5
4	SO4	A	3111	5/5	0.93	0.10	120,121,122,124	5
3	MES	A	3102	12/12	0.94	0.14	73,84,97,98	0
4	SO4	A	3105	5/5	0.95	0.08	130,132,133,134	0
2	MG	A	3101	1/1	0.98	0.10	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.



6.5 Other polymers [i](#)

There are no such residues in this entry.