W O R L D W I D E

wwPDB

P R O T E I N   D A T A   B A N K

wwPDB X-ray Structure Validation Summary Report (i)

Aug 28, 2023 – 10:40 PM EDT

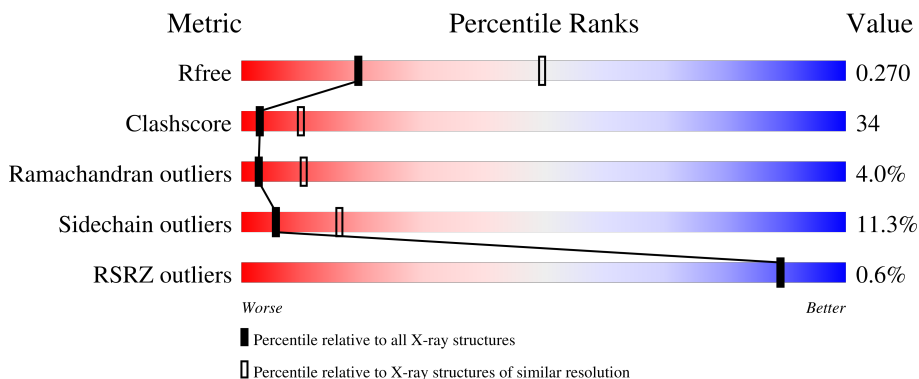|		
PDB ID	:	3ON0
Title	:	Crystal structure of the pED208 TraM-sbmA complex
Authors	:	Wong, J.J.W.; Lu, J.; Edwards, R.A.; Frost, L.S.; Mark Glover, J.N.
Deposited on	:	2010-08-27
Resolution	:	2.87 Å(reported)

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.87 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		0.270
Clashscore		34
Ramachandran outliers		4.0%
Sidechain outliers		11.3%
RSRZ outliers		0.6%

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$_{free}$	130704	2691 (2.90-2.86)
Clashscore	141614	2947 (2.90-2.86)
Ramachandran outliers	138981	2868 (2.90-2.86)
Sidechain outliers	138945	2871 (2.90-2.86)
RSRZ outliers	127900	2629 (2.90-2.86)

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	127	48% 39% 8% · 5%
1	B	127	47% 36% 9% · 7%
1	C	127	47% 37% 9% 7%
1	D	127	2% 45% 31% 9% 16%
2	P	24	8% 63% 29%

2 Entry composition ⓘ

There are 2 unique types of molecules in this entry. The entry contains 4226 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 Protein traM.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	121	Total	C	N	O	S	0	0	0
			979	616	161	195	7			
1	B	118	Total	C	N	O	S	0	0	0
			950	600	160	183	7			
1	C	118	Total	C	N	O	S	0	0	0
			950	600	160	183	7			
1	D	107	Total	C	N	O	S	0	0	0
			858	544	143	165	6			

- Molecule 2 is a DNA chain called sbmA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	P	24	Total	C	N	O	P	0	0	0
			489	236	88	142	23			

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.
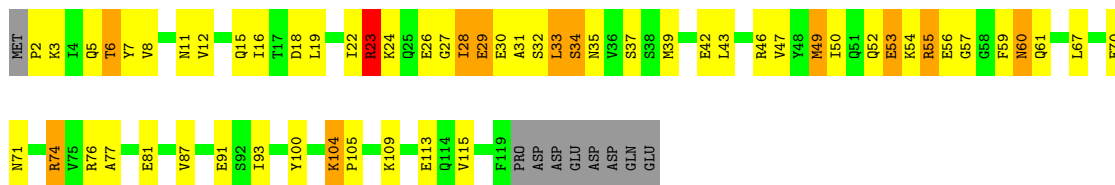
• Molecule 1: Protein traM

Chain A:
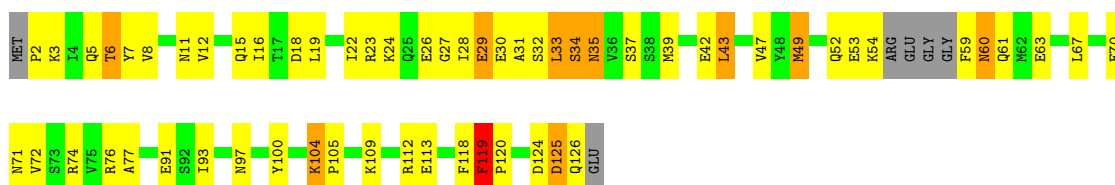
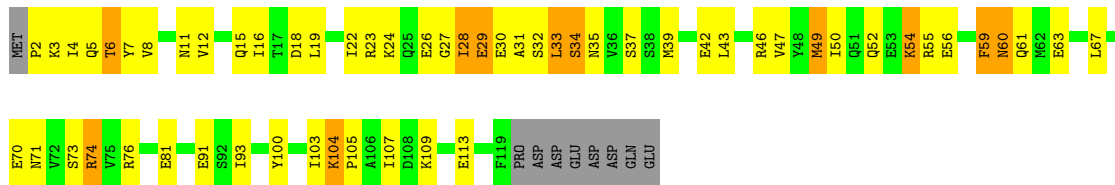• Molecule 1: Protein traM

Chain B:

• Molecule 1: Protein traM

Chain C:

• Molecule 1: Protein traM

Chain D:

L69 E70 N71 V72 S73 R74 V75 R76 Q90 I93 Y100 K104 P105 A106 I107 D108 K109 E113 F119 PRO ASP ASP GLU ASP ASP GLN GLU

• Molecule 2: sbmA

Chain P: 8%   63%   29%

A1 G2 A3 T4 T5 C6 G7 A8 A9 T10 C11 T12 A13 G14 A15 T16 T17 C18 G19 A20 A21 T22 C23 T24

4   Data and refinement statistics   (i)

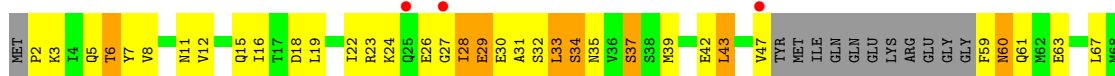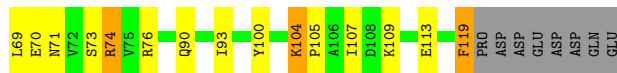| Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	93.03Å 154.69Å 167.56Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	83.78 – 2.87	Depositor
	45.74 – 2.87	EDS
% Data completeness	98.6 (83.78-2.87)	Depositor
(in resolution range)	98.6 (45.74-2.87)	EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	1.23 (at 2.86Å)	Xtriage
Refinement program	REFMAC 5.5.0066	Depositor
R, R_{free}	0.250 , 0.278	Depositor
	0.246 , 0.270	DCC
R_{free} test set	1383 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	72.6	Xtriage
Anisotropy	0.545	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 40.1	EDS
L-test for twinning[2]	$< |L| > = 0.50, < L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.008 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.021 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	4226	wwPDB-VP
Average B, all atoms (Å^2)	78.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.14% of the height of the origin peak. No significant pseudotranslation is detected.*

---

[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)

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	0.68	1/990 (0.1%)	0.64	0/1331
1	B	0.54	0/961	0.79	3/1290 (0.2%)
1	C	0.56	0/961	0.69	0/1290
1	D	0.54	0/867	0.65	0/1165
2	P	1.02	1/548 (0.2%)	2.01	21/844 (2.5%)
All	All	0.66	2/4327 (0.0%)	1.00	24/5920 (0.4%)

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	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	119	PHE	C-N	13.25	1.59	1.34
2	P	18	DC	C3'-O3'	-5.89	1.36	1.44

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	P	18	DC	O4'-C1'-N1	-12.43	99.30	108.00
1	B	23	ARG	NE-CZ-NH2	12.29	126.44	120.30
1	B	23	ARG	NE-CZ-NH1	-11.96	114.32	120.30
2	P	17	DT	O4'-C1'-N1	-10.63	100.56	108.00
2	P	9	DA	O4'-C1'-N9	-9.53	101.33	108.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	119	PHE	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	979	0	973	84	2
1	B	950	0	962	82	0
1	C	950	0	962	77	1
1	D	858	0	872	75	0
2	P	489	0	274	35	0
All	All	4226	0	4043	283	2

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 34.

The worst 5 of 283 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:P:1:DA:O5'	2:P:1:DA:C8	1.75	1.39
2:P:1:DA:O5'	2:P:1:DA:H8	1.06	1.24
2:P:24:DT:H3'	2:P:24:DT:C6	1.83	1.14
1:C:59:PHE:O	1:C:60:ASN:HB2	1.43	1.10
1:A:53:GLU:O	1:A:54:LYS:HG3	1.50	1.10

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:97:ASN:ND2	1:A:112:ARG:NH1[4_555]	1.92	0.28
1:A:109:LYS:NZ	1:C:81:GLU:OE1[4_555]	2.16	0.04

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	117/127 (92%)	101 (86%)	12 (10%)	4 (3%)	3	13
1	B	116/127 (91%)	96 (83%)	15 (13%)	5 (4%)	2	9
1	C	116/127 (91%)	98 (84%)	12 (10%)	6 (5%)	2	6
1	D	103/127 (81%)	92 (89%)	8 (8%)	3 (3%)	4	16
All	All	452/508 (89%)	387 (86%)	47 (10%)	18 (4%)	3	10

5 of 18 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	28	ILE
1	B	28	ILE
1	B	55	ARG
1	B	56	GLU
1	C	28	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	112/116 (97%)	101 (90%)	11 (10%)	8	22
1	B	107/116 (92%)	94 (88%)	13 (12%)	5	13
1	C	107/116 (92%)	95 (89%)	12 (11%)	6	16
1	D	98/116 (84%)	86 (88%)	12 (12%)	5	13
All	All	424/464 (91%)	376 (89%)	48 (11%)	6	16

5 of 48 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	43	LEU
1	C	104	LYS
1	C	49	MET
1	C	73	SER
1	D	33	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	97	ASN
1	D	65	ASN
1	D	97	ASN
1	D	90	GLN
1	B	35	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

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	121/127 (95%)	0.04	0	100	100	46, 73, 135, 170	0
1	B	118/127 (92%)	-0.04	0	100	100	51, 82, 119, 144	0
1	C	118/127 (92%)	-0.13	0	100	100	48, 73, 105, 118	0
1	D	107/127 (84%)	-0.05	3 (2%)	53	50	51, 67, 103, 123	0
2	P	24/24 (100%)	-0.58	0	100	100	60, 71, 107, 133	0
All	All	488/532 (91%)	-0.07	3 (0%)	89	89	46, 74, 116, 170	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	27	GLY	3.4
1	D	47	VAL	2.2
1	D	25	GLN	2.1

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 ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.