



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 27, 2020 – 02:08 PM BST

PDB ID : 6VDF
Title : Structure of the periplasmic domain of YejM from Salmonella typhimurium (twinned)
Authors : Gabale, U.; Ressler, S.
Deposited on : 2019-12-25
Resolution : 1.92 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 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 : 2.13
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) : 2.13

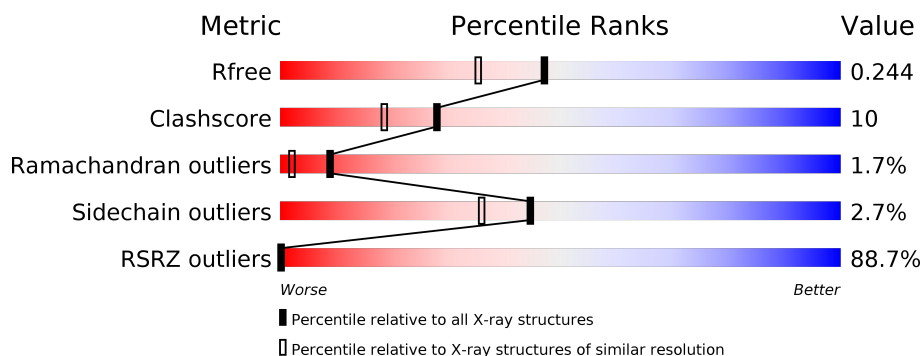
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.92 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	7937 (1.94-1.90)
Clashscore	141614	8644 (1.94-1.90)
Ramachandran outliers	138981	8530 (1.94-1.90)
Sidechain outliers	138945	8530 (1.94-1.90)
RSRZ outliers	127900	7793 (1.94-1.90)

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	368	<div> <div>80%</div> <div> <div>72%</div> <div>20%</div> <div>7%</div> </div> </div>
1	B	368	<div> <div>87%</div> <div> <div>71%</div> <div>21%</div> <div>7%</div> </div> </div>
1	C	368	<div> <div>83%</div> <div> <div>73%</div> <div>19%</div> <div>7%</div> </div> </div>
1	D	368	<div> <div>80%</div> <div> <div>71%</div> <div>21%</div> <div>7%</div> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	PGE	A	601	-	-	-	X
3	PEG	A	602	-	-	-	X
5	MN	B	602	-	-	-	X

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 22294 atoms, of which 10549 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 Periplasmic domain of the cardiolipin transporter protein YejM/PbgA.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	343	Total	C	H	N	O	S	0	0	0
			5341	1712	2623	476	522	8			
1	B	343	Total	C	H	N	O	S	0	0	0
			5342	1712	2624	476	522	8			
1	C	343	Total	C	H	N	O	S	0	0	0
			5341	1712	2623	476	522	8			
1	D	343	Total	C	H	N	O	S	0	0	0
			5341	1712	2623	476	522	8			

There are 88 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	219	MET	-	expression tag	UNP A0A5K1U4E1
A	220	SER	-	expression tag	UNP A0A5K1U4E1
A	221	GLY	-	expression tag	UNP A0A5K1U4E1
A	222	HIS	-	expression tag	UNP A0A5K1U4E1
A	223	HIS	-	expression tag	UNP A0A5K1U4E1
A	224	HIS	-	expression tag	UNP A0A5K1U4E1
A	225	HIS	-	expression tag	UNP A0A5K1U4E1
A	226	HIS	-	expression tag	UNP A0A5K1U4E1
A	227	HIS	-	expression tag	UNP A0A5K1U4E1
A	228	SER	-	expression tag	UNP A0A5K1U4E1
A	229	SER	-	expression tag	UNP A0A5K1U4E1
A	230	GLY	-	expression tag	UNP A0A5K1U4E1
A	231	LEU	-	expression tag	UNP A0A5K1U4E1
A	232	VAL	-	expression tag	UNP A0A5K1U4E1
A	233	PRO	-	expression tag	UNP A0A5K1U4E1
A	234	ARG	-	expression tag	UNP A0A5K1U4E1
A	235	GLY	-	expression tag	UNP A0A5K1U4E1
A	236	SER	-	expression tag	UNP A0A5K1U4E1
A	237	HIS	-	expression tag	UNP A0A5K1U4E1
A	238	MET	-	expression tag	UNP A0A5K1U4E1

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Chain	Residue	Modelled	Actual	Comment	Reference
A	239	ALA	-	expression tag	UNP A0A5K1U4E1
A	240	SER	-	expression tag	UNP A0A5K1U4E1
B	219	MET	-	expression tag	UNP A0A5K1U4E1
B	220	SER	-	expression tag	UNP A0A5K1U4E1
B	221	GLY	-	expression tag	UNP A0A5K1U4E1
B	222	HIS	-	expression tag	UNP A0A5K1U4E1
B	223	HIS	-	expression tag	UNP A0A5K1U4E1
B	224	HIS	-	expression tag	UNP A0A5K1U4E1
B	225	HIS	-	expression tag	UNP A0A5K1U4E1
B	226	HIS	-	expression tag	UNP A0A5K1U4E1
B	227	HIS	-	expression tag	UNP A0A5K1U4E1
B	228	SER	-	expression tag	UNP A0A5K1U4E1
B	229	SER	-	expression tag	UNP A0A5K1U4E1
B	230	GLY	-	expression tag	UNP A0A5K1U4E1
B	231	LEU	-	expression tag	UNP A0A5K1U4E1
B	232	VAL	-	expression tag	UNP A0A5K1U4E1
B	233	PRO	-	expression tag	UNP A0A5K1U4E1
B	234	ARG	-	expression tag	UNP A0A5K1U4E1
B	235	GLY	-	expression tag	UNP A0A5K1U4E1
B	236	SER	-	expression tag	UNP A0A5K1U4E1
B	237	HIS	-	expression tag	UNP A0A5K1U4E1
B	238	MET	-	expression tag	UNP A0A5K1U4E1
B	239	ALA	-	expression tag	UNP A0A5K1U4E1
B	240	SER	-	expression tag	UNP A0A5K1U4E1
C	219	MET	-	expression tag	UNP A0A5K1U4E1
C	220	SER	-	expression tag	UNP A0A5K1U4E1
C	221	GLY	-	expression tag	UNP A0A5K1U4E1
C	222	HIS	-	expression tag	UNP A0A5K1U4E1
C	223	HIS	-	expression tag	UNP A0A5K1U4E1
C	224	HIS	-	expression tag	UNP A0A5K1U4E1
C	225	HIS	-	expression tag	UNP A0A5K1U4E1
C	226	HIS	-	expression tag	UNP A0A5K1U4E1
C	227	HIS	-	expression tag	UNP A0A5K1U4E1
C	228	SER	-	expression tag	UNP A0A5K1U4E1
C	229	SER	-	expression tag	UNP A0A5K1U4E1
C	230	GLY	-	expression tag	UNP A0A5K1U4E1
C	231	LEU	-	expression tag	UNP A0A5K1U4E1
C	232	VAL	-	expression tag	UNP A0A5K1U4E1
C	233	PRO	-	expression tag	UNP A0A5K1U4E1
C	234	ARG	-	expression tag	UNP A0A5K1U4E1
C	235	GLY	-	expression tag	UNP A0A5K1U4E1
C	236	SER	-	expression tag	UNP A0A5K1U4E1

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Chain	Residue	Modelled	Actual	Comment	Reference
C	237	HIS	-	expression tag	UNP A0A5K1U4E1
C	238	MET	-	expression tag	UNP A0A5K1U4E1
C	239	ALA	-	expression tag	UNP A0A5K1U4E1
C	240	SER	-	expression tag	UNP A0A5K1U4E1
D	219	MET	-	expression tag	UNP A0A5K1U4E1
D	220	SER	-	expression tag	UNP A0A5K1U4E1
D	221	GLY	-	expression tag	UNP A0A5K1U4E1
D	222	HIS	-	expression tag	UNP A0A5K1U4E1
D	223	HIS	-	expression tag	UNP A0A5K1U4E1
D	224	HIS	-	expression tag	UNP A0A5K1U4E1
D	225	HIS	-	expression tag	UNP A0A5K1U4E1
D	226	HIS	-	expression tag	UNP A0A5K1U4E1
D	227	HIS	-	expression tag	UNP A0A5K1U4E1
D	228	SER	-	expression tag	UNP A0A5K1U4E1
D	229	SER	-	expression tag	UNP A0A5K1U4E1
D	230	GLY	-	expression tag	UNP A0A5K1U4E1
D	231	LEU	-	expression tag	UNP A0A5K1U4E1
D	232	VAL	-	expression tag	UNP A0A5K1U4E1
D	233	PRO	-	expression tag	UNP A0A5K1U4E1
D	234	ARG	-	expression tag	UNP A0A5K1U4E1
D	235	GLY	-	expression tag	UNP A0A5K1U4E1
D	236	SER	-	expression tag	UNP A0A5K1U4E1
D	237	HIS	-	expression tag	UNP A0A5K1U4E1
D	238	MET	-	expression tag	UNP A0A5K1U4E1
D	239	ALA	-	expression tag	UNP A0A5K1U4E1
D	240	SER	-	expression tag	UNP A0A5K1U4E1

- Molecule 2 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: C₆H₁₄O₄).



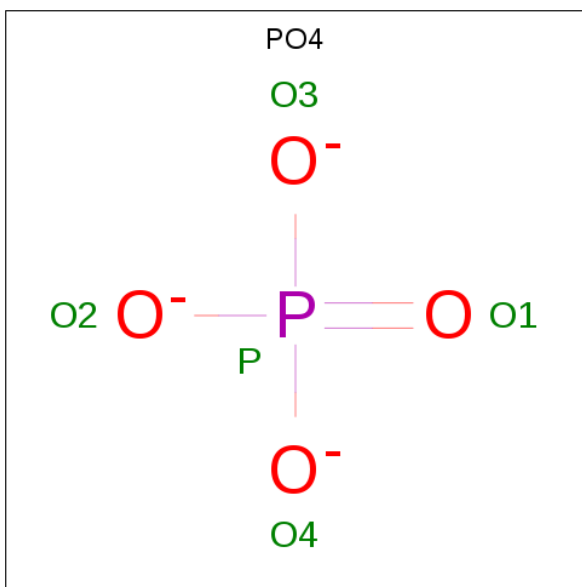
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	H	O	0	0
			24	6	14	4		

- Molecule 3 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O	0	0
			17	4	10	3		
3	D	1	Total	C	H	O	0	0
			17	4	10	3		

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



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

- Molecule 5 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

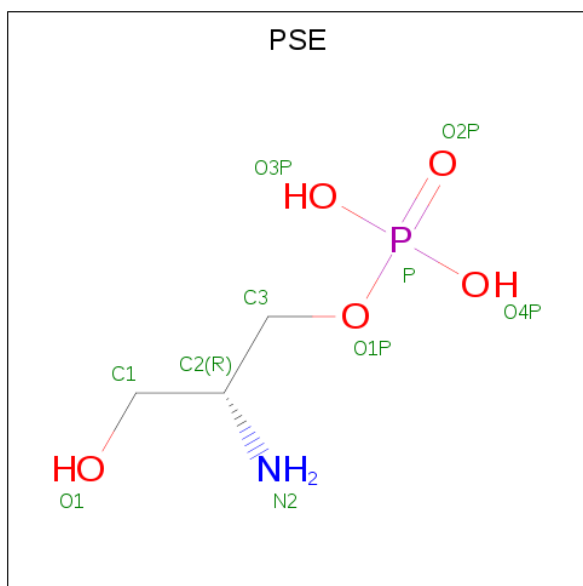
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Mn	0	0
			1	1		
5	A	1	Total	Mn	0	0
			1	1		
5	D	1	Total	Mn	0	0
			1	1		

- Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	B	1	Total	C	H	O	0	0
			10	2	6	2		

- Molecule 7 is O-PHOSPHOETHANOLAMINE (three-letter code: PSE) (formula: $C_3H_{10}NO_5P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	C	1	Total	C	H	N	O	P	
			18	3	8	1	5	1	0
7	D	1	Total	C	H	N	O	P	
			18	3	8	1	5	1	0

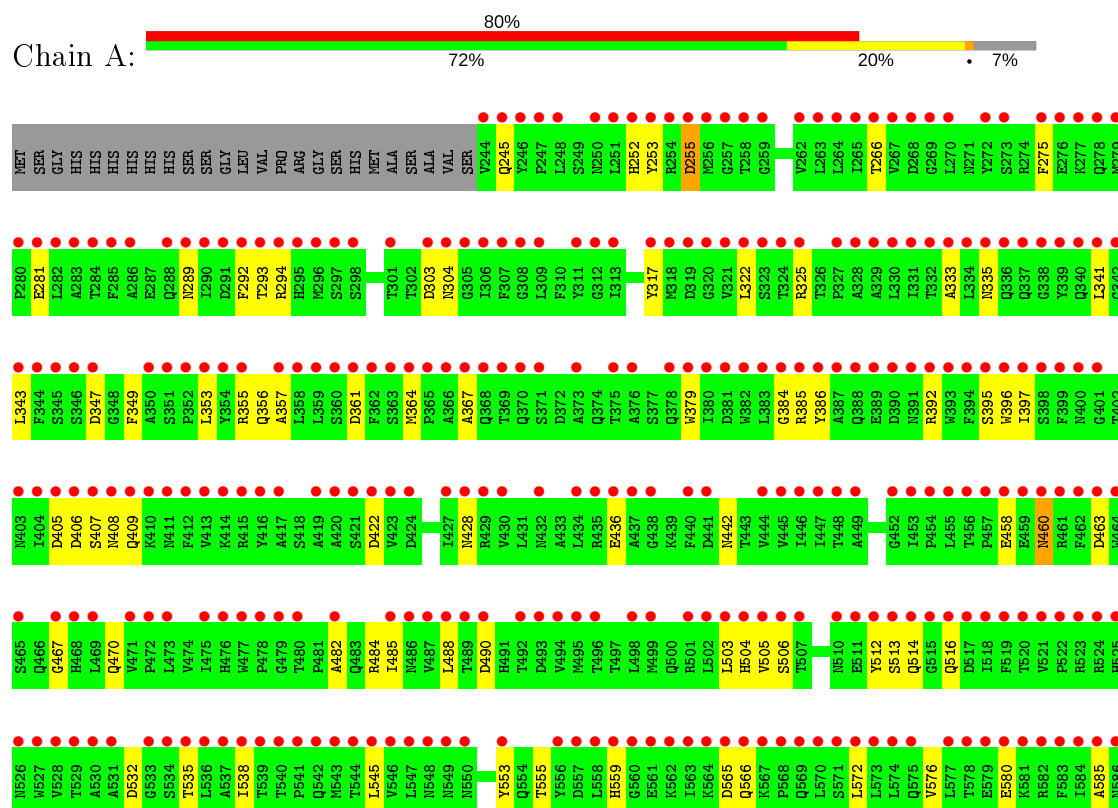
- Molecule 8 is water.

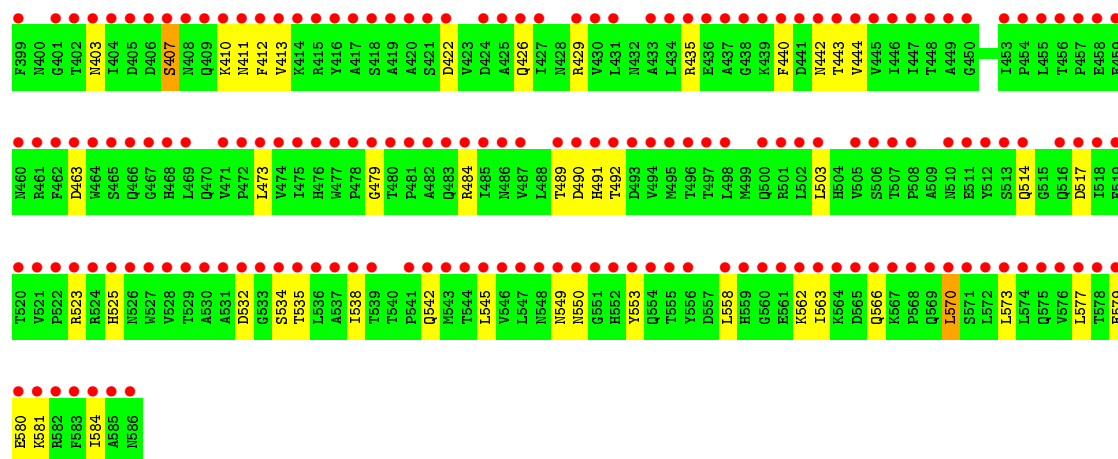
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	183	Total 183	O 183	0	0
8	B	199	Total 199	O 199	0	0
8	C	194	Total 194	O 194	0	0
8	D	236	Total 236	O 236	0	0

3 Residue-property plots

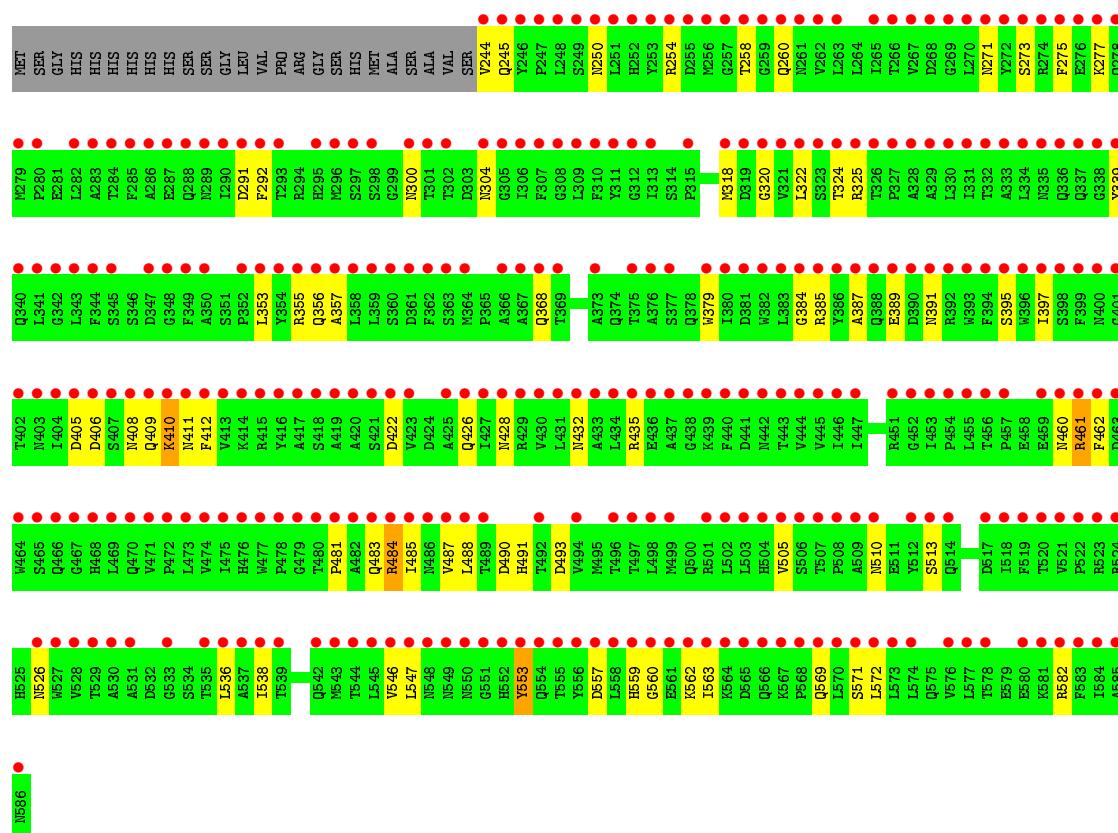
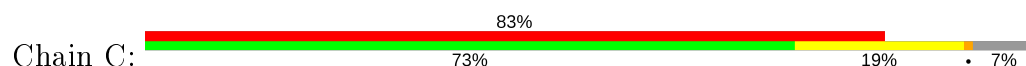
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Periplasmic domain of the cardiolipin transporter protein YejM/PbgA

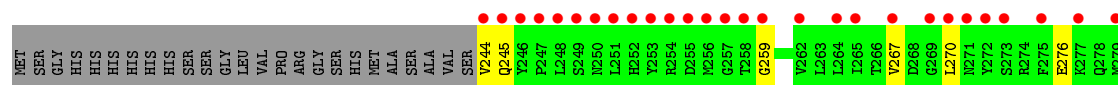
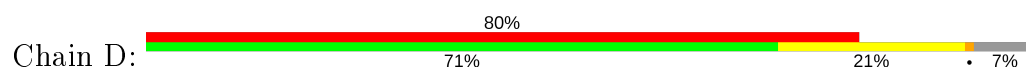


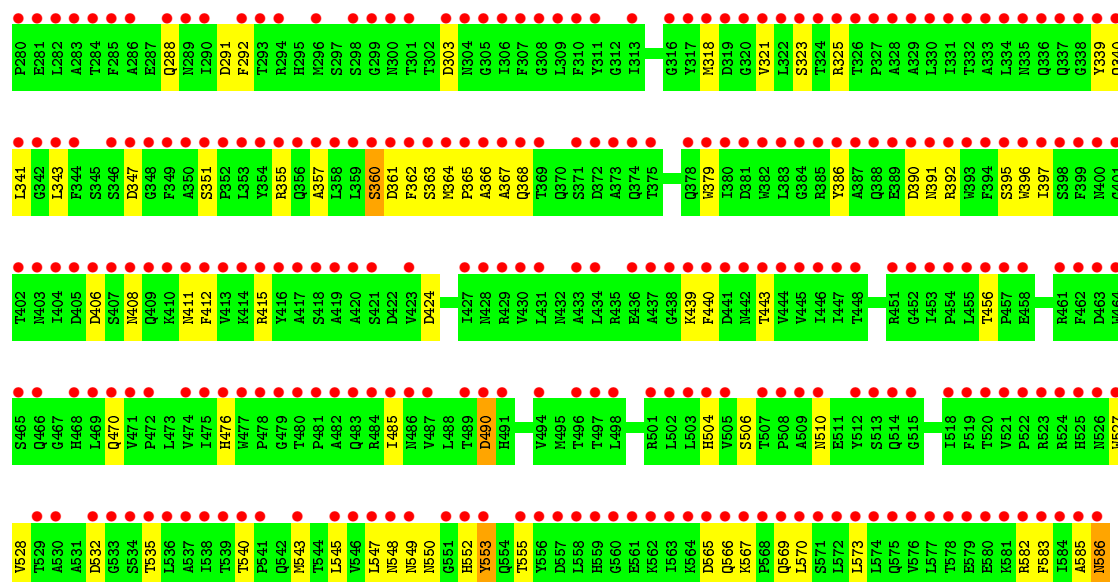


- Molecule 1: Periplasmic domain of the cardiolipin transporter protein YejM/PbgA



- Molecule 1: Periplasmic domain of the cardiolipin transporter protein YejM/PbgA





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	42.95Å 42.96Å 181.21Å 94.28° 94.02° 111.78°	Depositor
Resolution (Å)	59.90 – 1.92 59.90 – 1.92	Depositor EDS
% Data completeness (in resolution range)	77.2 (59.90-1.92) 76.1 (59.90-1.92)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	15.55 (at 1.92Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.211 , 0.261 0.198 , 0.244	Depositor DCC
R_{free} test set	3268 reflections (4.65%)	wwPDB-VP
Wilson B-factor (Å ²)	19.6	Xtriage
Anisotropy	0.431	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 27.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.428 for k,h,-h-k-l 0.388 for -k,-h,l 0.387 for -h,-k,h+k+l	Xtriage
Reported twinning fraction	0.450 for -h,-k,h+k+l	Depositor
Outliers	0 of 70265 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	22294	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.56% 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: PGE, PO4, MN, EDO, PSE, PEG

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	0.24	0/2782	0.43	0/3790
1	B	0.24	0/2782	0.43	0/3790
1	C	0.24	0/2782	0.42	0/3790
1	D	0.24	0/2782	0.42	0/3790
All	All	0.24	0/11128	0.42	0/15160

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	2718	2623	2623	52	1
1	B	2718	2624	2623	55	2
1	C	2718	2623	2623	52	3
1	D	2718	2623	2623	55	0
2	A	10	14	14	0	0
3	A	7	10	10	0	0
3	D	7	10	10	0	0
4	A	5	0	0	0	0
4	D	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	D	1	0	0	0	0
6	B	4	6	6	0	0
7	C	10	8	8	0	0
7	D	10	8	8	0	0
8	A	183	0	0	31	2
8	B	199	0	0	29	4
8	C	194	0	0	26	3
8	D	236	0	0	25	6
All	All	11745	10549	10548	212	17

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 10.

The worst 5 of 212 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:C:526:ASN:OD1	8:C:701:HOH:O	1.93	0.86
1:C:462:PHE:O	8:C:702:HOH:O	1.97	0.82
1:A:513:SER:N	8:A:709:HOH:O	2.11	0.82
1:B:484:ARG:NH2	8:B:710:HOH:O	2.11	0.81
1:A:303:ASP:OD2	8:A:701:HOH:O	1.99	0.80

The worst 5 of 17 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:B:407:SER:OG	1:B:435:ARG:O[1_655]	1.90	0.30
1:C:322:LEU:O	1:C:484:ARG:NH2[1_655]	1.98	0.22
8:D:979:HOH:O	8:D:983:HOH:O[1_665]	2.04	0.16
8:B:852:HOH:O	8:B:878:HOH:O[1_445]	2.05	0.15
8:B:888:HOH:O	8:B:897:HOH:O[1_445]	2.06	0.14

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	341/368 (93%)	308 (90%)	29 (8%)	4 (1%)	13	4
1	B	341/368 (93%)	302 (89%)	31 (9%)	8 (2%)	6	1
1	C	341/368 (93%)	307 (90%)	27 (8%)	7 (2%)	7	1
1	D	341/368 (93%)	317 (93%)	20 (6%)	4 (1%)	13	4
All	All	1364/1472 (93%)	1234 (90%)	107 (8%)	23 (2%)	9	2

5 of 23 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	409	GLN
1	B	407	SER
1	B	410	LYS
1	C	410	LYS
1	D	367	ALA

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	295/315 (94%)	287 (97%)	8 (3%)	44	36
1	B	295/315 (94%)	285 (97%)	10 (3%)	37	27
1	C	295/315 (94%)	289 (98%)	6 (2%)	55	49
1	D	295/315 (94%)	287 (97%)	8 (3%)	44	36
All	All	1180/1260 (94%)	1148 (97%)	32 (3%)	44	36

5 of 32 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	550	ASN
1	B	570	LEU
1	D	553	TYR
1	B	562	LYS
1	C	275	PHE

Some 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	370	GLN
1	B	391	ASN
1	C	468	HIS
1	B	260	GLN
1	C	428	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 ⓘ

Of 11 ligands modelled in this entry, 3 are monoatomic - leaving 8 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	PEG	A	602	-	6,6,6	0.48	0	5,5,5	0.43	0
6	EDO	B	601	-	3,3,3	0.76	0	2,2,2	0.55	0
7	PSE	C	601	-	9,9,9	0.85	0	9,12,12	0.68	0
3	PEG	D	702	-	6,6,6	0.49	0	5,5,5	0.47	0
4	PO4	A	603	-	4,4,4	0.91	0	6,6,6	0.43	0
7	PSE	D	701	-	9,9,9	0.84	0	9,12,12	0.68	0
2	PGE	A	601	-	9,9,9	0.31	0	8,8,8	0.35	0
4	PO4	D	703	-	4,4,4	0.93	0	6,6,6	0.44	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	PEG	A	602	-	-	2/4/4/4	-
6	EDO	B	601	-	-	1/1/1/1	-
7	PSE	C	601	-	-	5/8/8/8	-
3	PEG	D	702	-	-	1/4/4/4	-
7	PSE	D	701	-	-	4/8/8/8	-
2	PGE	A	601	-	-	3/7/7/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 16 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	601	EDO	O1-C1-C2-O2
7	C	601	PSE	O1-C1-C2-N2
7	C	601	PSE	O1-C1-C2-C3
7	C	601	PSE	C3-O1P-P-O3P
7	C	601	PSE	C3-O1P-P-O4P

There are no ring outliers.

No monomer is involved in short contacts.

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 [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	343/368 (93%)	3.76	295 (86%) 0 0	9, 17, 36, 52	0
1	B	343/368 (93%)	4.33	320 (93%) 0 0	11, 19, 34, 64	0
1	C	343/368 (93%)	4.09	307 (89%) 0 0	11, 18, 35, 52	0
1	D	343/368 (93%)	3.84	295 (86%) 0 0	9, 16, 36, 52	0
All	All	1372/1472 (93%)	4.01	1217 (88%) 0 0	9, 18, 36, 64	0

The worst 5 of 1217 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	366	ALA	20.5
1	A	386	TYR	16.9
1	D	391	ASN	14.8
1	C	404	ILE	14.7
1	B	343	LEU	13.4

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
2	PGE	A	601	10/10	0.19	0.54	36,43,44,44	0
5	MN	B	602	1/1	0.33	0.42	65,65,65,65	0
5	MN	D	704	1/1	0.34	0.31	67,67,67,67	0
3	PEG	A	602	7/7	0.36	0.49	43,52,53,53	0
7	PSE	C	601	10/10	0.39	0.38	49,50,59,59	0
6	EDO	B	601	4/4	0.47	0.34	44,53,53,53	0
5	MN	A	604	1/1	0.59	0.19	45,45,45,45	0
4	PO4	A	603	5/5	0.63	0.35	54,54,54,54	0
3	PEG	D	702	7/7	0.66	0.34	43,51,52,52	0
7	PSE	D	701	10/10	0.67	0.32	43,45,54,55	0
4	PO4	D	703	5/5	0.70	0.33	62,64,64,65	0

6.5 Other polymers [i](#)

There are no such residues in this entry.