



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 24, 2020 – 02:58 PM BST

PDB ID : 6VAT
Title : Structure of the periplasmic domain of YejM from Salmonella typhimurium
Authors : Gabale, U.; Ressler, S.
Deposited on : 2019-12-17
Resolution : 2.35 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
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) : 2.13

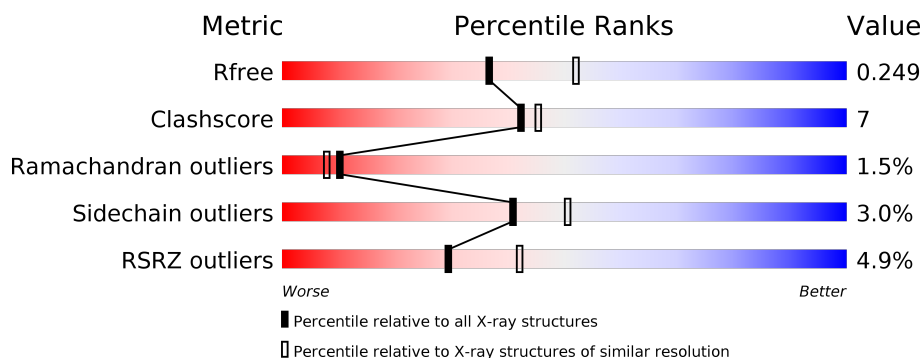
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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	1164 (2.36-2.36)
Clashscore	141614	1232 (2.36-2.36)
Ramachandran outliers	138981	1211 (2.36-2.36)
Sidechain outliers	138945	1212 (2.36-2.36)
RSRZ outliers	127900	1150 (2.36-2.36)

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>4%</div> <div> <div></div> <div>81%</div> <div>12%</div> <div>• 7%</div> </div> </div>
1	B	368	<div> <div>%</div> <div> <div></div> <div>82%</div> <div>11%</div> <div>• 7%</div> </div> </div>
1	C	368	<div> <div>2%</div> <div> <div></div> <div>81%</div> <div>12%</div> <div>• 6%</div> </div> </div>
1	D	368	<div> <div>%</div> <div> <div></div> <div>80%</div> <div>12%</div> <div>• 7%</div> </div> </div>
1	E	368	<div> <div>7%</div> <div> <div></div> <div>70%</div> <div>22%</div> <div>•• 6%</div> </div> </div>
1	F	368	<div> <div>13%</div> <div> <div></div> <div>69%</div> <div>23%</div> <div>• 6%</div> </div> </div>

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 17290 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 Periplasmic domain of the cardiolipin transporter protein YejM/PbgA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	344	Total	C	N	O	S	0	0	0
			2723	1716	476	523	8			
1	B	343	Total	C	N	O	S	0	0	0
			2716	1711	475	522	8			
1	C	345	Total	C	N	O	S	0	1	0
			2734	1723	478	525	8			
1	D	343	Total	C	N	O	S	0	0	0
			2718	1712	476	522	8			
1	E	346	Total	C	N	O	S	0	0	0
			2736	1723	479	526	8			
1	F	345	Total	C	N	O	S	0	0	0
			2731	1720	478	525	8			

There are 132 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	219	MET	-	expression tag	UNP A0A4V1IDU5
A	220	SER	-	expression tag	UNP A0A4V1IDU5
A	221	GLY	-	expression tag	UNP A0A4V1IDU5
A	222	HIS	-	expression tag	UNP A0A4V1IDU5
A	223	HIS	-	expression tag	UNP A0A4V1IDU5
A	224	HIS	-	expression tag	UNP A0A4V1IDU5
A	225	HIS	-	expression tag	UNP A0A4V1IDU5
A	226	HIS	-	expression tag	UNP A0A4V1IDU5
A	227	HIS	-	expression tag	UNP A0A4V1IDU5
A	228	SER	-	expression tag	UNP A0A4V1IDU5
A	229	SER	-	expression tag	UNP A0A4V1IDU5
A	230	GLY	-	expression tag	UNP A0A4V1IDU5
A	231	LEU	-	expression tag	UNP A0A4V1IDU5
A	232	VAL	-	expression tag	UNP A0A4V1IDU5
A	233	PRO	-	expression tag	UNP A0A4V1IDU5
A	234	ARG	-	expression tag	UNP A0A4V1IDU5

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Chain	Residue	Modelled	Actual	Comment	Reference
A	235	GLY	-	expression tag	UNP A0A4V1IDU5
A	236	SER	-	expression tag	UNP A0A4V1IDU5
A	237	HIS	-	expression tag	UNP A0A4V1IDU5
A	238	MET	-	expression tag	UNP A0A4V1IDU5
A	239	ALA	-	expression tag	UNP A0A4V1IDU5
A	240	SER	-	expression tag	UNP A0A4V1IDU5
B	219	MET	-	expression tag	UNP A0A4V1IDU5
B	220	SER	-	expression tag	UNP A0A4V1IDU5
B	221	GLY	-	expression tag	UNP A0A4V1IDU5
B	222	HIS	-	expression tag	UNP A0A4V1IDU5
B	223	HIS	-	expression tag	UNP A0A4V1IDU5
B	224	HIS	-	expression tag	UNP A0A4V1IDU5
B	225	HIS	-	expression tag	UNP A0A4V1IDU5
B	226	HIS	-	expression tag	UNP A0A4V1IDU5
B	227	HIS	-	expression tag	UNP A0A4V1IDU5
B	228	SER	-	expression tag	UNP A0A4V1IDU5
B	229	SER	-	expression tag	UNP A0A4V1IDU5
B	230	GLY	-	expression tag	UNP A0A4V1IDU5
B	231	LEU	-	expression tag	UNP A0A4V1IDU5
B	232	VAL	-	expression tag	UNP A0A4V1IDU5
B	233	PRO	-	expression tag	UNP A0A4V1IDU5
B	234	ARG	-	expression tag	UNP A0A4V1IDU5
B	235	GLY	-	expression tag	UNP A0A4V1IDU5
B	236	SER	-	expression tag	UNP A0A4V1IDU5
B	237	HIS	-	expression tag	UNP A0A4V1IDU5
B	238	MET	-	expression tag	UNP A0A4V1IDU5
B	239	ALA	-	expression tag	UNP A0A4V1IDU5
B	240	SER	-	expression tag	UNP A0A4V1IDU5
C	219	MET	-	expression tag	UNP A0A4V1IDU5
C	220	SER	-	expression tag	UNP A0A4V1IDU5
C	221	GLY	-	expression tag	UNP A0A4V1IDU5
C	222	HIS	-	expression tag	UNP A0A4V1IDU5
C	223	HIS	-	expression tag	UNP A0A4V1IDU5
C	224	HIS	-	expression tag	UNP A0A4V1IDU5
C	225	HIS	-	expression tag	UNP A0A4V1IDU5
C	226	HIS	-	expression tag	UNP A0A4V1IDU5
C	227	HIS	-	expression tag	UNP A0A4V1IDU5
C	228	SER	-	expression tag	UNP A0A4V1IDU5
C	229	SER	-	expression tag	UNP A0A4V1IDU5
C	230	GLY	-	expression tag	UNP A0A4V1IDU5
C	231	LEU	-	expression tag	UNP A0A4V1IDU5
C	232	VAL	-	expression tag	UNP A0A4V1IDU5

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Chain	Residue	Modelled	Actual	Comment	Reference
C	233	PRO	-	expression tag	UNP A0A4V1IDU5
C	234	ARG	-	expression tag	UNP A0A4V1IDU5
C	235	GLY	-	expression tag	UNP A0A4V1IDU5
C	236	SER	-	expression tag	UNP A0A4V1IDU5
C	237	HIS	-	expression tag	UNP A0A4V1IDU5
C	238	MET	-	expression tag	UNP A0A4V1IDU5
C	239	ALA	-	expression tag	UNP A0A4V1IDU5
C	240	SER	-	expression tag	UNP A0A4V1IDU5
D	219	MET	-	expression tag	UNP A0A4V1IDU5
D	220	SER	-	expression tag	UNP A0A4V1IDU5
D	221	GLY	-	expression tag	UNP A0A4V1IDU5
D	222	HIS	-	expression tag	UNP A0A4V1IDU5
D	223	HIS	-	expression tag	UNP A0A4V1IDU5
D	224	HIS	-	expression tag	UNP A0A4V1IDU5
D	225	HIS	-	expression tag	UNP A0A4V1IDU5
D	226	HIS	-	expression tag	UNP A0A4V1IDU5
D	227	HIS	-	expression tag	UNP A0A4V1IDU5
D	228	SER	-	expression tag	UNP A0A4V1IDU5
D	229	SER	-	expression tag	UNP A0A4V1IDU5
D	230	GLY	-	expression tag	UNP A0A4V1IDU5
D	231	LEU	-	expression tag	UNP A0A4V1IDU5
D	232	VAL	-	expression tag	UNP A0A4V1IDU5
D	233	PRO	-	expression tag	UNP A0A4V1IDU5
D	234	ARG	-	expression tag	UNP A0A4V1IDU5
D	235	GLY	-	expression tag	UNP A0A4V1IDU5
D	236	SER	-	expression tag	UNP A0A4V1IDU5
D	237	HIS	-	expression tag	UNP A0A4V1IDU5
D	238	MET	-	expression tag	UNP A0A4V1IDU5
D	239	ALA	-	expression tag	UNP A0A4V1IDU5
D	240	SER	-	expression tag	UNP A0A4V1IDU5
E	219	MET	-	expression tag	UNP A0A4V1IDU5
E	220	SER	-	expression tag	UNP A0A4V1IDU5
E	221	GLY	-	expression tag	UNP A0A4V1IDU5
E	222	HIS	-	expression tag	UNP A0A4V1IDU5
E	223	HIS	-	expression tag	UNP A0A4V1IDU5
E	224	HIS	-	expression tag	UNP A0A4V1IDU5
E	225	HIS	-	expression tag	UNP A0A4V1IDU5
E	226	HIS	-	expression tag	UNP A0A4V1IDU5
E	227	HIS	-	expression tag	UNP A0A4V1IDU5
E	228	SER	-	expression tag	UNP A0A4V1IDU5
E	229	SER	-	expression tag	UNP A0A4V1IDU5
E	230	GLY	-	expression tag	UNP A0A4V1IDU5

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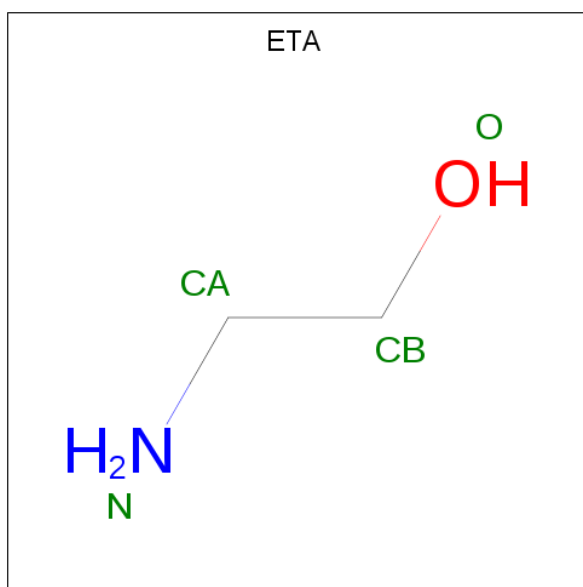
Chain	Residue	Modelled	Actual	Comment	Reference
E	231	LEU	-	expression tag	UNP A0A4V1IDU5
E	232	VAL	-	expression tag	UNP A0A4V1IDU5
E	233	PRO	-	expression tag	UNP A0A4V1IDU5
E	234	ARG	-	expression tag	UNP A0A4V1IDU5
E	235	GLY	-	expression tag	UNP A0A4V1IDU5
E	236	SER	-	expression tag	UNP A0A4V1IDU5
E	237	HIS	-	expression tag	UNP A0A4V1IDU5
E	238	MET	-	expression tag	UNP A0A4V1IDU5
E	239	ALA	-	expression tag	UNP A0A4V1IDU5
E	240	SER	-	expression tag	UNP A0A4V1IDU5
F	219	MET	-	expression tag	UNP A0A4V1IDU5
F	220	SER	-	expression tag	UNP A0A4V1IDU5
F	221	GLY	-	expression tag	UNP A0A4V1IDU5
F	222	HIS	-	expression tag	UNP A0A4V1IDU5
F	223	HIS	-	expression tag	UNP A0A4V1IDU5
F	224	HIS	-	expression tag	UNP A0A4V1IDU5
F	225	HIS	-	expression tag	UNP A0A4V1IDU5
F	226	HIS	-	expression tag	UNP A0A4V1IDU5
F	227	HIS	-	expression tag	UNP A0A4V1IDU5
F	228	SER	-	expression tag	UNP A0A4V1IDU5
F	229	SER	-	expression tag	UNP A0A4V1IDU5
F	230	GLY	-	expression tag	UNP A0A4V1IDU5
F	231	LEU	-	expression tag	UNP A0A4V1IDU5
F	232	VAL	-	expression tag	UNP A0A4V1IDU5
F	233	PRO	-	expression tag	UNP A0A4V1IDU5
F	234	ARG	-	expression tag	UNP A0A4V1IDU5
F	235	GLY	-	expression tag	UNP A0A4V1IDU5
F	236	SER	-	expression tag	UNP A0A4V1IDU5
F	237	HIS	-	expression tag	UNP A0A4V1IDU5
F	238	MET	-	expression tag	UNP A0A4V1IDU5
F	239	ALA	-	expression tag	UNP A0A4V1IDU5
F	240	SER	-	expression tag	UNP A0A4V1IDU5

- Molecule 2 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: C₈H₁₈O₅).



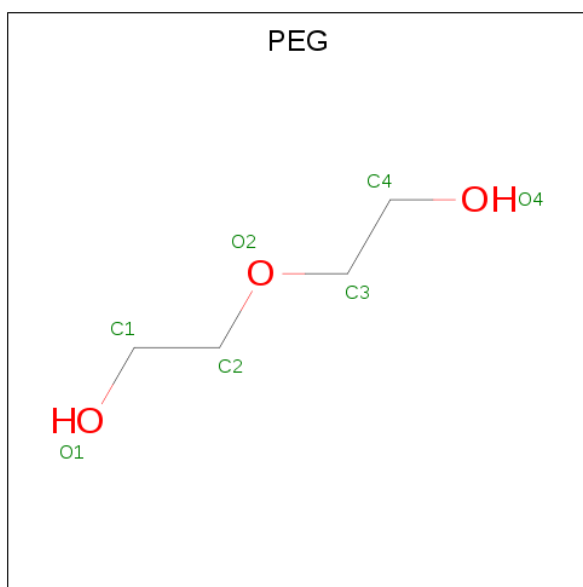
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			13	8	5		
2	A	1	Total	C	O	0	0
			13	8	5		
2	B	1	Total	C	O	0	0
			13	8	5		
2	C	1	Total	C	O	0	0
			13	8	5		
2	C	1	Total	C	O	0	0
			13	8	5		
2	D	1	Total	C	O	0	0
			13	8	5		
2	E	1	Total	C	O	0	0
			13	8	5		

- Molecule 3 is ETHANOLAMINE (three-letter code: ETA) (formula: C₂H₇NO).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			4	2	1	1		
3	C	1	Total	C	N	O	0	0
			4	2	1	1		
3	D	1	Total	C	N	O	0	0
			4	2	1	1		

- Molecule 4 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).



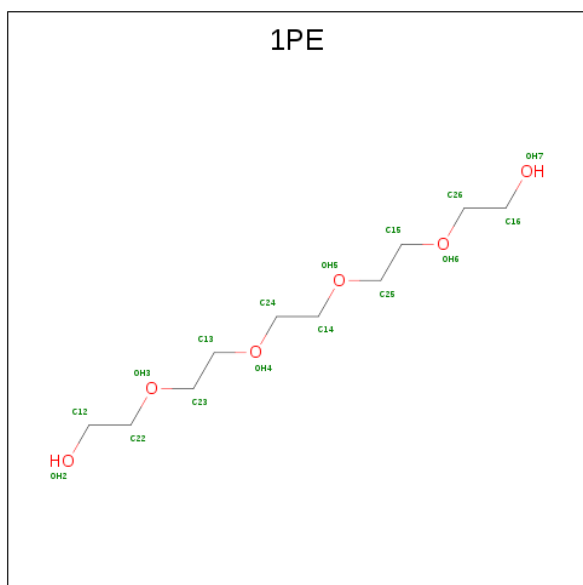
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			7	4	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	C	1	Total	C	O	0	0
			7	4	3		
4	D	1	Total	C	O	0	0
			7	4	3		

- Molecule 5 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: $C_{10}H_{22}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			16	10	6		
5	C	1	Total	C	O	0	0
			16	10	6		
5	E	1	Total	C	O	0	0
			16	10	6		
5	F	1	Total	C	O	0	0
			16	10	6		

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

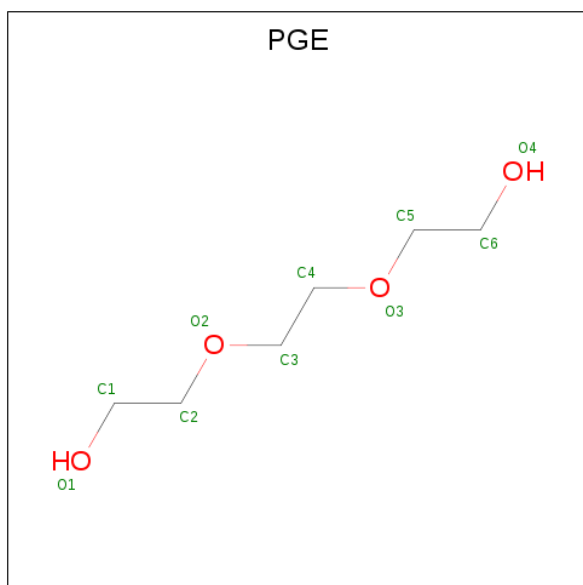
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total	Mg	0	0
			1	1		
6	A	1	Total	Mg	0	0
			1	1		
6	D	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	C	1	Total	Mg	0	0
			1	1		
6	F	1	Total	Mg	0	0
			1	1		

- Molecule 7 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).

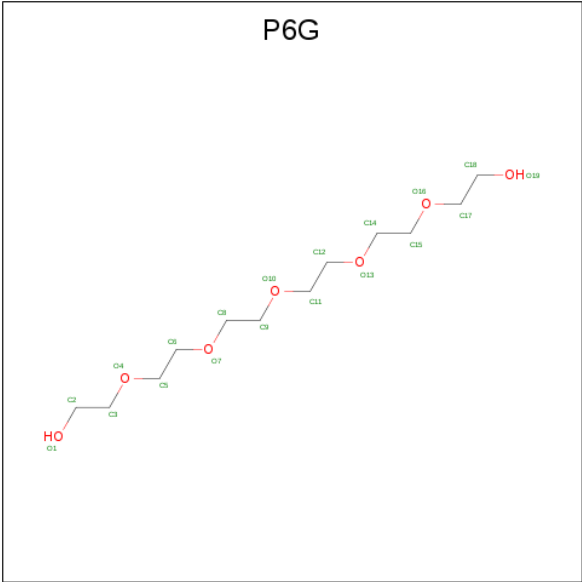


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	C	O	0	0
			10	6	4		
7	C	1	Total	C	O	0	0
			10	6	4		
7	F	1	Total	C	O	0	0
			10	6	4		

- Molecule 8 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	B	1	Total	Ca	0	0
			1	1		
8	C	1	Total	Ca	0	0
			1	1		
8	E	1	Total	Ca	0	0
			1	1		

- Molecule 9 is HEXAETHYLENE GLYCOL (three-letter code: P6G) (formula: $C_{12}H_{26}O_7$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	D	1	Total	C	O	0	0
			19	12	7		

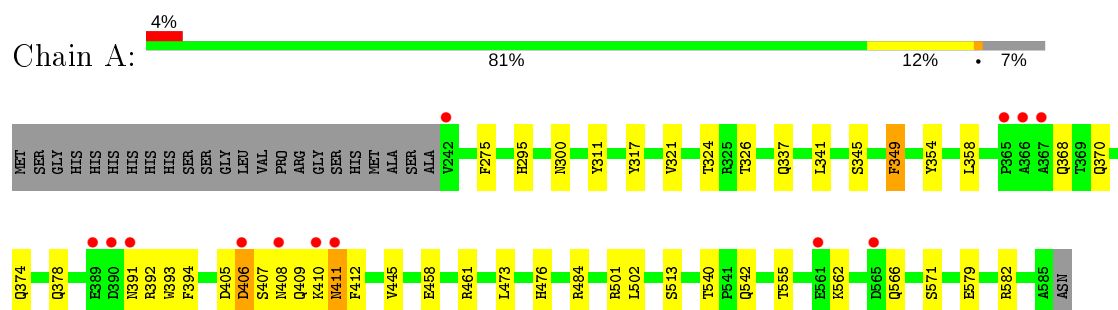
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	142	Total	O	0	0
			142	142		
10	B	151	Total	O	0	0
			151	151		
10	C	133	Total	O	0	0
			133	133		
10	D	141	Total	O	0	0
			141	141		
10	E	77	Total	O	0	0
			77	77		
10	F	43	Total	O	0	0
			43	43		

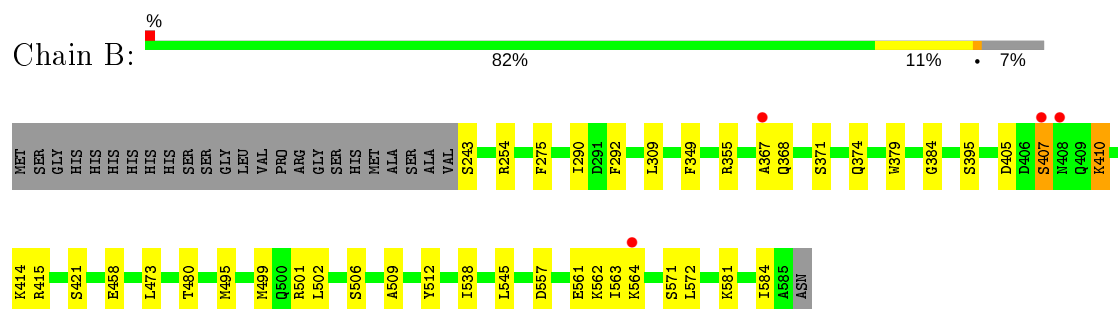
3 Residue-property plots

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.

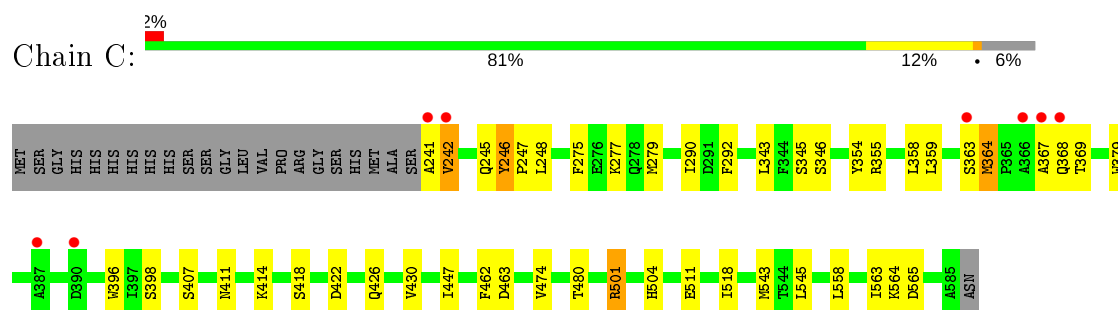
- Molecule 1: Periplasmic domain of the cardiolipin transporter protein YejM/PbgA



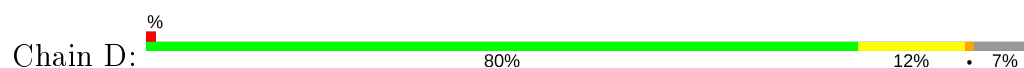
- Molecule 1: Periplasmic domain of the cardiolipin transporter protein YejM/PbgA

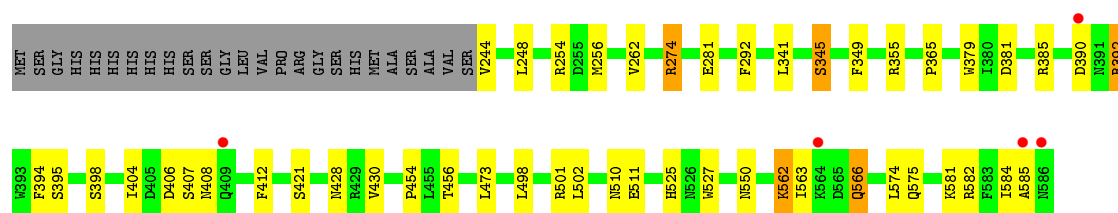


- Molecule 1: Periplasmic domain of the cardiolipin transporter protein YejM/PbgA

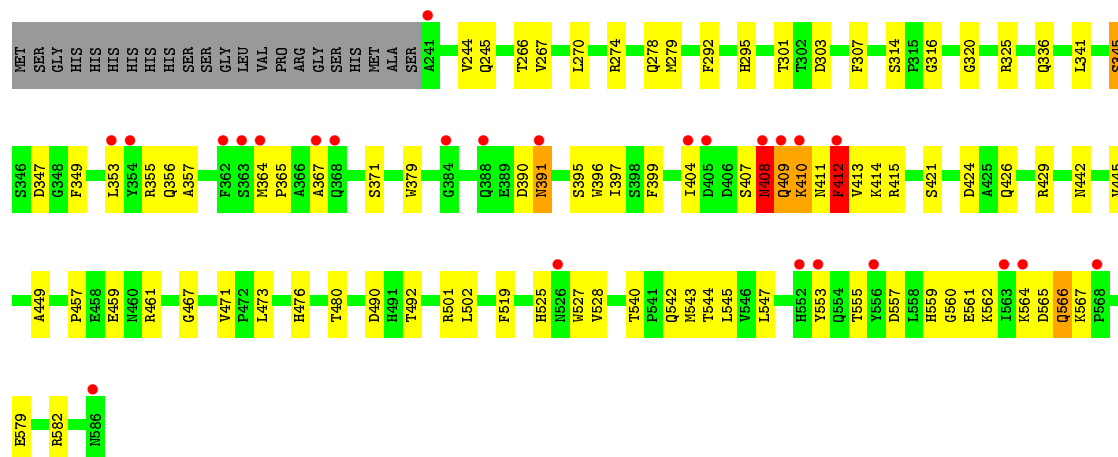


- Molecule 1: Periplasmic domain of the cardiolipin transporter protein YejM/PbgA

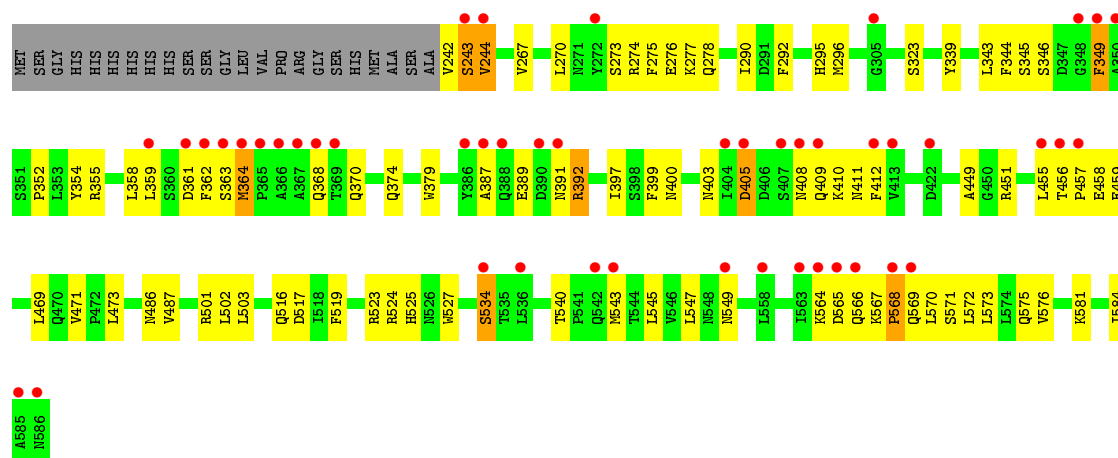




- Molecule 1: Periplasmic domain of the cardiolipin transporter protein YejM/PbgA



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	113.80Å 113.80Å 299.78Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	59.65 – 2.35 59.65 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.9 (59.65-2.35) 85.4 (59.65-2.20)	Depositor EDS
R_{merge}	0.21	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.30 (at 2.20Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.196 , 0.249 0.196 , 0.249	Depositor DCC
R_{free} test set	4744 reflections (4.18%)	wwPDB-VP
Wilson B-factor (Å ²)	23.6	Xtriage
Anisotropy	0.099	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 48.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.035 for -h,-k,l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	17290	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.99% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, PGE, CA, 1PE, PG4, ETA, P6G, 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	0.27	0/2787	0.47	0/3797
1	B	0.27	0/2780	0.44	0/3787
1	C	0.26	0/2801	0.45	0/3816
1	D	0.27	0/2782	0.44	0/3790
1	E	0.28	0/2800	0.47	0/3815
1	F	0.28	0/2795	0.47	0/3808
All	All	0.27	0/16745	0.46	0/22813

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	E	0	1
1	F	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	409	GLN	Peptide
1	F	565	ASP	Peptide

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	2723	0	2631	30	0
1	B	2716	0	2622	25	0
1	C	2734	0	2641	26	0
1	D	2718	0	2623	31	0
1	E	2736	0	2642	54	0
1	F	2731	0	2637	61	0
2	A	26	0	36	2	0
2	B	13	0	18	2	0
2	C	26	0	36	3	0
2	D	13	0	18	1	0
2	E	13	0	18	1	0
3	A	4	0	7	1	0
3	C	4	0	7	0	0
3	D	4	0	7	1	0
4	A	7	0	10	0	0
4	C	7	0	10	2	0
4	D	7	0	10	0	0
5	A	16	0	22	1	0
5	C	16	0	20	0	0
5	E	16	0	22	6	0
5	F	16	0	22	5	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
6	F	1	0	0	0	0
7	B	10	0	14	2	0
7	C	10	0	14	0	0
7	F	10	0	14	1	0
8	B	1	0	0	0	0
8	C	1	0	0	0	0
8	E	1	0	0	0	0
9	D	19	0	26	2	0
10	A	142	0	0	1	0
10	B	151	0	0	1	0
10	C	133	0	0	0	0
10	D	141	0	0	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	E	77	0	0	2	0
10	F	43	0	0	0	0
All	All	17290	0	16127	227	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 7.

The worst 5 of 227 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:458:GLU:HG3	1:A:461:ARG:NH2	1.74	1.01
1:A:458:GLU:CG	1:A:461:ARG:NH2	2.24	1.01
1:A:540:THR:HG22	1:A:542:GLN:H	1.34	0.91
1:A:458:GLU:HG3	1:A:461:ARG:CZ	2.06	0.85
1:E:501:ARG:HH12	5:E:602:IPE:H161	1.40	0.85

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	342/368 (93%)	318 (93%)	21 (6%)	3 (1%)	17	17
1	B	341/368 (93%)	323 (95%)	16 (5%)	2 (1%)	25	27
1	C	344/368 (94%)	313 (91%)	25 (7%)	6 (2%)	9	7
1	D	341/368 (93%)	325 (95%)	13 (4%)	3 (1%)	17	17
1	E	344/368 (94%)	318 (92%)	19 (6%)	7 (2%)	7	5
1	F	343/368 (93%)	296 (86%)	37 (11%)	10 (3%)	4	2
All	All	2055/2208 (93%)	1893 (92%)	131 (6%)	31 (2%)	10	8

5 of 31 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	406	ASP
1	C	242	VAL
1	E	412	PHE
1	C	369	THR
1	D	585	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	296/315 (94%)	287 (97%)	9 (3%)	41	50
1	B	295/315 (94%)	288 (98%)	7 (2%)	49	59
1	C	297/315 (94%)	290 (98%)	7 (2%)	49	59
1	D	295/315 (94%)	287 (97%)	8 (3%)	44	55
1	E	297/315 (94%)	285 (96%)	12 (4%)	31	39
1	F	297/315 (94%)	286 (96%)	11 (4%)	34	42
All	All	1777/1890 (94%)	1723 (97%)	54 (3%)	41	50

5 of 54 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	274	ARG
1	D	575	GLN
1	F	361	ASP
1	D	345	SER
1	D	395	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 17 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	408	ASN
1	E	411	ASN

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Mol	Chain	Res	Type
1	F	525	HIS
1	E	356	GLN
1	F	549	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 29 ligands modelled in this entry, 8 are monoatomic - leaving 21 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	$\# Z > 2$
5	1PE	C	606	1	15,15,15	0.54	0	14,14,14	0.42	0
2	PG4	A	602	-	12,12,12	0.53	0	11,11,11	0.22	0
5	1PE	E	602	-	15,15,15	0.53	0	14,14,14	0.55	0
3	ETA	A	603	-	3,3,3	0.51	0	2,2,2	0.35	0
4	PEG	A	604	-	6,6,6	0.48	0	5,5,5	0.28	0
7	PGE	B	602	-	9,9,9	0.51	0	8,8,8	0.21	0
2	PG4	C	602	-	12,12,12	0.53	0	11,11,11	0.25	0
2	PG4	B	601	-	12,12,12	0.51	0	11,11,11	0.21	0
3	ETA	C	604	-	3,3,3	0.49	0	2,2,2	0.54	0
2	PG4	D	601	-	12,12,12	0.52	0	11,11,11	0.23	0
2	PG4	A	601	-	12,12,12	0.52	0	11,11,11	0.20	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	P6G	D	604	-	18,18,18	0.53	0	17,17,17	0.39	0
7	PGE	F	701	-	9,9,9	0.51	0	8,8,8	0.23	0
5	1PE	F	702	-	15,15,15	0.54	0	14,14,14	0.43	0
7	PGE	C	603	-	9,9,9	0.51	0	8,8,8	0.23	0
3	ETA	D	602	-	3,3,3	0.52	0	2,2,2	0.47	0
2	PG4	E	601	-	12,12,12	0.53	0	11,11,11	0.22	0
4	PEG	C	605	-	6,6,6	0.49	0	5,5,5	0.30	0
4	PEG	D	603	-	6,6,6	0.49	0	5,5,5	0.30	0
5	1PE	A	605	-	15,15,15	0.53	0	14,14,14	0.45	0
2	PG4	C	601	-	12,12,12	0.52	0	11,11,11	0.26	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
5	1PE	C	606	1	-	8/13/13/13	-
2	PG4	A	602	-	-	4/10/10/10	-
5	1PE	E	602	-	-	7/13/13/13	-
3	ETA	A	603	-	-	0/1/1/1	-
4	PEG	A	604	-	-	2/4/4/4	-
7	PGE	B	602	-	-	4/7/7/7	-
2	PG4	C	602	-	-	7/10/10/10	-
2	PG4	B	601	-	-	9/10/10/10	-
3	ETA	C	604	-	-	0/1/1/1	-
2	PG4	D	601	-	-	4/10/10/10	-
2	PG4	A	601	-	-	4/10/10/10	-
9	P6G	D	604	-	-	11/16/16/16	-
7	PGE	F	701	-	-	3/7/7/7	-
5	1PE	F	702	-	-	9/13/13/13	-
7	PGE	C	603	-	-	4/7/7/7	-
3	ETA	D	602	-	-	1/1/1/1	-
2	PG4	E	601	-	-	4/10/10/10	-
4	PEG	C	605	-	-	2/4/4/4	-
4	PEG	D	603	-	-	2/4/4/4	-
5	1PE	A	605	-	-	9/13/13/13	-
2	PG4	C	601	-	-	4/10/10/10	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 98 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	602	ETA	N-CA-CB-O
9	D	604	P6G	O1-C2-C3-O4
5	A	605	1PE	C24-C14-OH5-C25
5	A	605	1PE	OH4-C13-C23-OH3
5	F	702	1PE	OH4-C13-C23-OH3

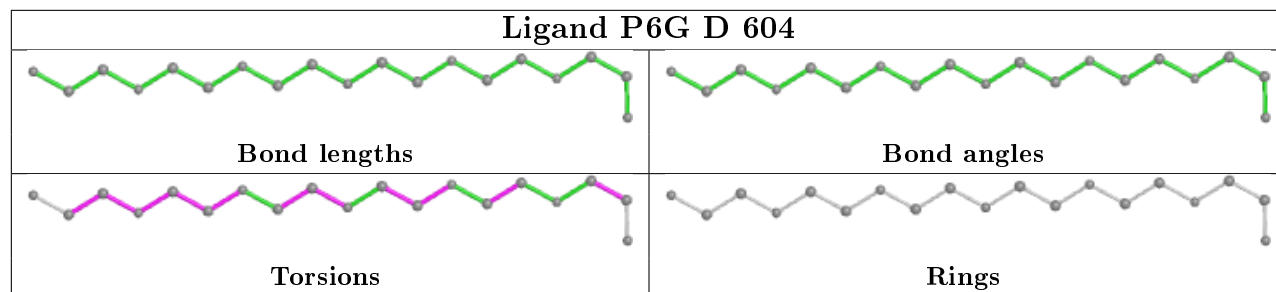
There are no ring outliers.

15 monomers are involved in 30 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	E	602	1PE	6	0
3	A	603	ETA	1	0
7	B	602	PGE	2	0
2	C	602	PG4	2	0
2	B	601	PG4	2	0
2	D	601	PG4	1	0
2	A	601	PG4	2	0
9	D	604	P6G	2	0
7	F	701	PGE	1	0
5	F	702	1PE	5	0
3	D	602	ETA	1	0
2	E	601	PG4	1	0
4	C	605	PEG	2	0
5	A	605	1PE	1	0
2	C	601	PG4	1	0

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 than 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.



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	344/368 (93%)	-0.21	13 (3%) 40 53	17, 36, 104, 160	0
1	B	343/368 (93%)	-0.40	4 (1%) 79 86	21, 36, 73, 109	0
1	C	345/368 (93%)	-0.28	8 (2%) 60 70	24, 38, 79, 128	0
1	D	343/368 (93%)	-0.36	5 (1%) 73 81	22, 39, 79, 117	0
1	E	346/368 (94%)	0.30	25 (7%) 15 23	30, 62, 122, 182	0
1	F	345/368 (93%)	0.72	47 (13%) 3 4	32, 68, 141, 178	0
All	All	2066/2208 (93%)	-0.04	102 (4%) 29 42	17, 44, 110, 182	0

The worst 5 of 102 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	386	TYR	13.4
1	F	566	GLN	8.4
1	F	366	ALA	7.8
1	F	407	SER	6.4
1	E	563	ILE	6.2

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 ⓘ

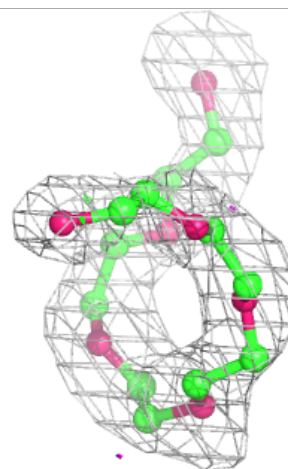
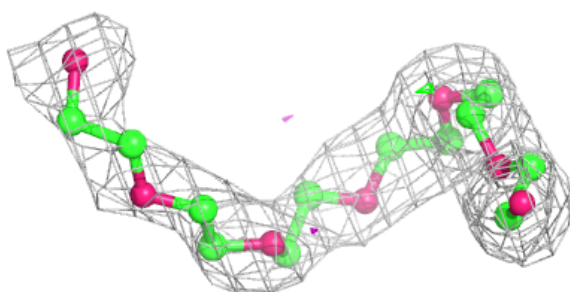
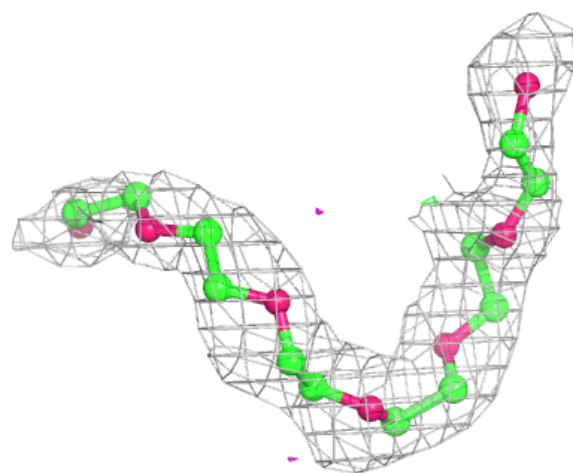
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	PG4	C	602	13/13	0.66	0.26	58,69,81,82	0
8	CA	E	603	1/1	0.69	0.26	174,174,174,174	0
7	PGE	F	701	10/10	0.71	0.22	76,79,80,80	0
4	PEG	C	605	7/7	0.74	0.24	48,60,70,72	0
3	ETA	A	603	4/4	0.75	0.28	53,58,64,66	0
7	PGE	C	603	10/10	0.75	0.18	67,68,68,69	0
2	PG4	D	601	13/13	0.76	0.13	57,68,73,74	0
7	PGE	B	602	10/10	0.77	0.15	41,68,73,73	0
2	PG4	A	602	13/13	0.78	0.16	56,64,72,73	0
2	PG4	E	601	13/13	0.79	0.18	69,71,74,74	0
4	PEG	A	604	7/7	0.80	0.28	69,74,76,77	0
4	PEG	D	603	7/7	0.80	0.14	63,67,70,70	0
5	1PE	F	702	16/16	0.85	0.16	55,63,70,71	0
9	P6G	D	604	19/19	0.85	0.18	49,63,70,71	0
5	1PE	E	602	16/16	0.86	0.14	50,57,60,62	0
3	ETA	C	604	4/4	0.87	0.14	25,33,38,39	0
2	PG4	B	601	13/13	0.88	0.12	40,47,54,60	0
3	ETA	D	602	4/4	0.88	0.17	47,51,52,54	0
5	1PE	A	605	16/16	0.88	0.11	49,60,66,66	0
2	PG4	A	601	13/13	0.89	0.15	43,52,58,61	0
5	1PE	C	606	16/16	0.90	0.13	45,54,59,62	0
6	MG	F	703	1/1	0.93	0.06	49,49,49,49	0
2	PG4	C	601	13/13	0.93	0.13	43,49,59,62	0
6	MG	C	607	1/1	0.94	0.20	35,35,35,35	0
8	CA	B	604	1/1	0.96	0.06	60,60,60,60	0
6	MG	A	606	1/1	0.97	0.11	26,26,26,26	0
6	MG	B	603	1/1	0.97	0.11	30,30,30,30	0
6	MG	D	605	1/1	0.98	0.10	37,37,37,37	0
8	CA	C	608	1/1	0.99	0.07	53,53,53,53	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 P6G D 604:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.