



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 27, 2020 – 02:17 PM BST

PDB ID : 6VC7  
Title : Structure of the F349A mutant of the periplasmic domain of YejM from *Salmonella typhimurium*  
Authors : Gabale, U.; Ressler, S.  
Deposited on : 2019-12-20  
Resolution : 2.05 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](mailto: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.

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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

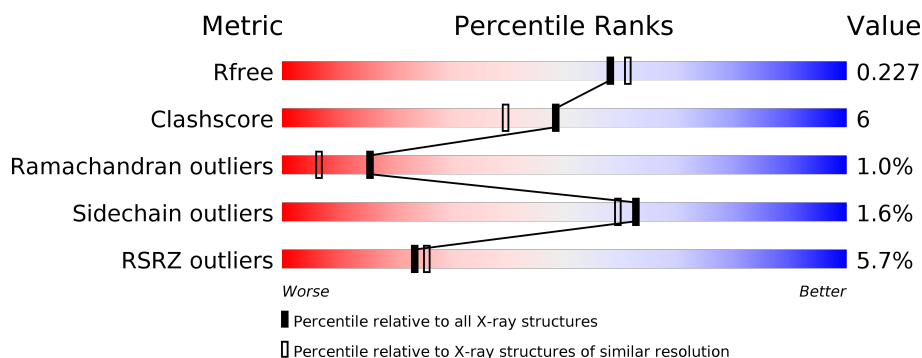
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.05 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	1692 (2.04-2.04)
Clashscore	141614	1773 (2.04-2.04)
Ramachandran outliers	138981	1752 (2.04-2.04)
Sidechain outliers	138945	1752 (2.04-2.04)
RSRZ outliers	127900	1672 (2.04-2.04)

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  $\geq 3$ , 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>6%</div> <div> <div></div> <div>81%</div> <div>12%</div> <div>7%</div> </div> </div>
1	B	368	<div> <div>5%</div> <div> <div></div> <div>83%</div> <div>11%</div> <div>7%</div> </div> </div>
1	C	368	<div> <div>4%</div> <div> <div></div> <div>79%</div> <div>13%</div> <div>7%</div> </div> </div>
1	D	368	<div> <div>5%</div> <div> <div></div> <div>78%</div> <div>15%</div> <div>7%</div> </div> </div>
1	E	368	<div> <div>6%</div> <div> <div></div> <div>82%</div> <div>10%</div> <div>7%</div> </div> </div>
1	F	368	<div> <div>6%</div> <div> <div></div> <div>80%</div> <div>13%</div> <div>7%</div> </div> </div>

## 2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 17703 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	2	0
			2727	1715	478	526	8			
1	B	344	Total	C	N	O	S	0	3	0
			2727	1715	477	527	8			
1	C	344	Total	C	N	O	S	0	3	0
			2727	1715	477	527	8			
1	D	344	Total	C	N	O	S	0	3	0
			2727	1715	477	527	8			
1	E	344	Total	C	N	O	S	0	1	0
			2721	1711	477	525	8			
1	F	344	Total	C	N	O	S	0	2	0
			2724	1713	477	526	8			

There are 138 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	219	MET	-	expression tag	UNP A0A5A8TP41
A	220	SER	-	expression tag	UNP A0A5A8TP41
A	221	GLY	-	expression tag	UNP A0A5A8TP41
A	222	HIS	-	expression tag	UNP A0A5A8TP41
A	223	HIS	-	expression tag	UNP A0A5A8TP41
A	224	HIS	-	expression tag	UNP A0A5A8TP41
A	225	HIS	-	expression tag	UNP A0A5A8TP41
A	226	HIS	-	expression tag	UNP A0A5A8TP41
A	227	HIS	-	expression tag	UNP A0A5A8TP41
A	228	SER	-	expression tag	UNP A0A5A8TP41
A	229	SER	-	expression tag	UNP A0A5A8TP41
A	230	GLY	-	expression tag	UNP A0A5A8TP41
A	231	LEU	-	expression tag	UNP A0A5A8TP41
A	232	VAL	-	expression tag	UNP A0A5A8TP41
A	233	PRO	-	expression tag	UNP A0A5A8TP41
A	234	ARG	-	expression tag	UNP A0A5A8TP41

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Chain	Residue	Modelled	Actual	Comment	Reference
A	235	GLY	-	expression tag	UNP A0A5A8TP41
A	236	SER	-	expression tag	UNP A0A5A8TP41
A	237	HIS	-	expression tag	UNP A0A5A8TP41
A	238	MET	-	expression tag	UNP A0A5A8TP41
A	239	ALA	-	expression tag	UNP A0A5A8TP41
A	240	SER	-	expression tag	UNP A0A5A8TP41
A	349	ALA	PHE	engineered mutation	UNP A0A5A8TP41
B	219	MET	-	expression tag	UNP A0A5A8TP41
B	220	SER	-	expression tag	UNP A0A5A8TP41
B	221	GLY	-	expression tag	UNP A0A5A8TP41
B	222	HIS	-	expression tag	UNP A0A5A8TP41
B	223	HIS	-	expression tag	UNP A0A5A8TP41
B	224	HIS	-	expression tag	UNP A0A5A8TP41
B	225	HIS	-	expression tag	UNP A0A5A8TP41
B	226	HIS	-	expression tag	UNP A0A5A8TP41
B	227	HIS	-	expression tag	UNP A0A5A8TP41
B	228	SER	-	expression tag	UNP A0A5A8TP41
B	229	SER	-	expression tag	UNP A0A5A8TP41
B	230	GLY	-	expression tag	UNP A0A5A8TP41
B	231	LEU	-	expression tag	UNP A0A5A8TP41
B	232	VAL	-	expression tag	UNP A0A5A8TP41
B	233	PRO	-	expression tag	UNP A0A5A8TP41
B	234	ARG	-	expression tag	UNP A0A5A8TP41
B	235	GLY	-	expression tag	UNP A0A5A8TP41
B	236	SER	-	expression tag	UNP A0A5A8TP41
B	237	HIS	-	expression tag	UNP A0A5A8TP41
B	238	MET	-	expression tag	UNP A0A5A8TP41
B	239	ALA	-	expression tag	UNP A0A5A8TP41
B	240	SER	-	expression tag	UNP A0A5A8TP41
B	349	ALA	PHE	engineered mutation	UNP A0A5A8TP41
C	219	MET	-	expression tag	UNP A0A5A8TP41
C	220	SER	-	expression tag	UNP A0A5A8TP41
C	221	GLY	-	expression tag	UNP A0A5A8TP41
C	222	HIS	-	expression tag	UNP A0A5A8TP41
C	223	HIS	-	expression tag	UNP A0A5A8TP41
C	224	HIS	-	expression tag	UNP A0A5A8TP41
C	225	HIS	-	expression tag	UNP A0A5A8TP41
C	226	HIS	-	expression tag	UNP A0A5A8TP41
C	227	HIS	-	expression tag	UNP A0A5A8TP41
C	228	SER	-	expression tag	UNP A0A5A8TP41
C	229	SER	-	expression tag	UNP A0A5A8TP41
C	230	GLY	-	expression tag	UNP A0A5A8TP41

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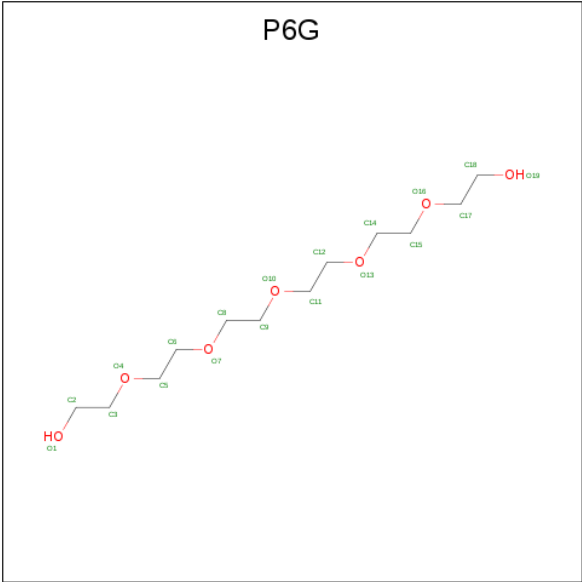
Chain	Residue	Modelled	Actual	Comment	Reference
C	231	LEU	-	expression tag	UNP A0A5A8TP41
C	232	VAL	-	expression tag	UNP A0A5A8TP41
C	233	PRO	-	expression tag	UNP A0A5A8TP41
C	234	ARG	-	expression tag	UNP A0A5A8TP41
C	235	GLY	-	expression tag	UNP A0A5A8TP41
C	236	SER	-	expression tag	UNP A0A5A8TP41
C	237	HIS	-	expression tag	UNP A0A5A8TP41
C	238	MET	-	expression tag	UNP A0A5A8TP41
C	239	ALA	-	expression tag	UNP A0A5A8TP41
C	240	SER	-	expression tag	UNP A0A5A8TP41
C	349	ALA	PHE	engineered mutation	UNP A0A5A8TP41
D	219	MET	-	expression tag	UNP A0A5A8TP41
D	220	SER	-	expression tag	UNP A0A5A8TP41
D	221	GLY	-	expression tag	UNP A0A5A8TP41
D	222	HIS	-	expression tag	UNP A0A5A8TP41
D	223	HIS	-	expression tag	UNP A0A5A8TP41
D	224	HIS	-	expression tag	UNP A0A5A8TP41
D	225	HIS	-	expression tag	UNP A0A5A8TP41
D	226	HIS	-	expression tag	UNP A0A5A8TP41
D	227	HIS	-	expression tag	UNP A0A5A8TP41
D	228	SER	-	expression tag	UNP A0A5A8TP41
D	229	SER	-	expression tag	UNP A0A5A8TP41
D	230	GLY	-	expression tag	UNP A0A5A8TP41
D	231	LEU	-	expression tag	UNP A0A5A8TP41
D	232	VAL	-	expression tag	UNP A0A5A8TP41
D	233	PRO	-	expression tag	UNP A0A5A8TP41
D	234	ARG	-	expression tag	UNP A0A5A8TP41
D	235	GLY	-	expression tag	UNP A0A5A8TP41
D	236	SER	-	expression tag	UNP A0A5A8TP41
D	237	HIS	-	expression tag	UNP A0A5A8TP41
D	238	MET	-	expression tag	UNP A0A5A8TP41
D	239	ALA	-	expression tag	UNP A0A5A8TP41
D	240	SER	-	expression tag	UNP A0A5A8TP41
D	349	ALA	PHE	engineered mutation	UNP A0A5A8TP41
E	219	MET	-	expression tag	UNP A0A5A8TP41
E	220	SER	-	expression tag	UNP A0A5A8TP41
E	221	GLY	-	expression tag	UNP A0A5A8TP41
E	222	HIS	-	expression tag	UNP A0A5A8TP41
E	223	HIS	-	expression tag	UNP A0A5A8TP41
E	224	HIS	-	expression tag	UNP A0A5A8TP41
E	225	HIS	-	expression tag	UNP A0A5A8TP41
E	226	HIS	-	expression tag	UNP A0A5A8TP41

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Chain	Residue	Modelled	Actual	Comment	Reference
E	227	HIS	-	expression tag	UNP A0A5A8TP41
E	228	SER	-	expression tag	UNP A0A5A8TP41
E	229	SER	-	expression tag	UNP A0A5A8TP41
E	230	GLY	-	expression tag	UNP A0A5A8TP41
E	231	LEU	-	expression tag	UNP A0A5A8TP41
E	232	VAL	-	expression tag	UNP A0A5A8TP41
E	233	PRO	-	expression tag	UNP A0A5A8TP41
E	234	ARG	-	expression tag	UNP A0A5A8TP41
E	235	GLY	-	expression tag	UNP A0A5A8TP41
E	236	SER	-	expression tag	UNP A0A5A8TP41
E	237	HIS	-	expression tag	UNP A0A5A8TP41
E	238	MET	-	expression tag	UNP A0A5A8TP41
E	239	ALA	-	expression tag	UNP A0A5A8TP41
E	240	SER	-	expression tag	UNP A0A5A8TP41
E	349	ALA	PHE	engineered mutation	UNP A0A5A8TP41
F	219	MET	-	expression tag	UNP A0A5A8TP41
F	220	SER	-	expression tag	UNP A0A5A8TP41
F	221	GLY	-	expression tag	UNP A0A5A8TP41
F	222	HIS	-	expression tag	UNP A0A5A8TP41
F	223	HIS	-	expression tag	UNP A0A5A8TP41
F	224	HIS	-	expression tag	UNP A0A5A8TP41
F	225	HIS	-	expression tag	UNP A0A5A8TP41
F	226	HIS	-	expression tag	UNP A0A5A8TP41
F	227	HIS	-	expression tag	UNP A0A5A8TP41
F	228	SER	-	expression tag	UNP A0A5A8TP41
F	229	SER	-	expression tag	UNP A0A5A8TP41
F	230	GLY	-	expression tag	UNP A0A5A8TP41
F	231	LEU	-	expression tag	UNP A0A5A8TP41
F	232	VAL	-	expression tag	UNP A0A5A8TP41
F	233	PRO	-	expression tag	UNP A0A5A8TP41
F	234	ARG	-	expression tag	UNP A0A5A8TP41
F	235	GLY	-	expression tag	UNP A0A5A8TP41
F	236	SER	-	expression tag	UNP A0A5A8TP41
F	237	HIS	-	expression tag	UNP A0A5A8TP41
F	238	MET	-	expression tag	UNP A0A5A8TP41
F	239	ALA	-	expression tag	UNP A0A5A8TP41
F	240	SER	-	expression tag	UNP A0A5A8TP41
F	349	ALA	PHE	engineered mutation	UNP A0A5A8TP41

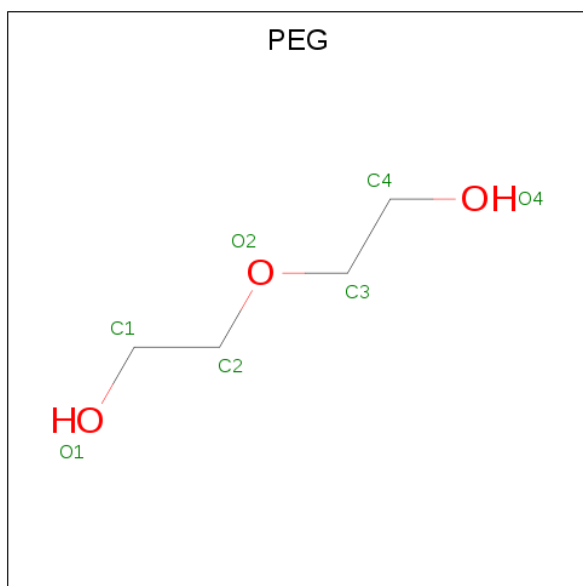
- Molecule 2 is HEXAETHYLENE GLYCOL (three-letter code: P6G) (formula: C<sub>12</sub>H<sub>26</sub>O<sub>7</sub>).



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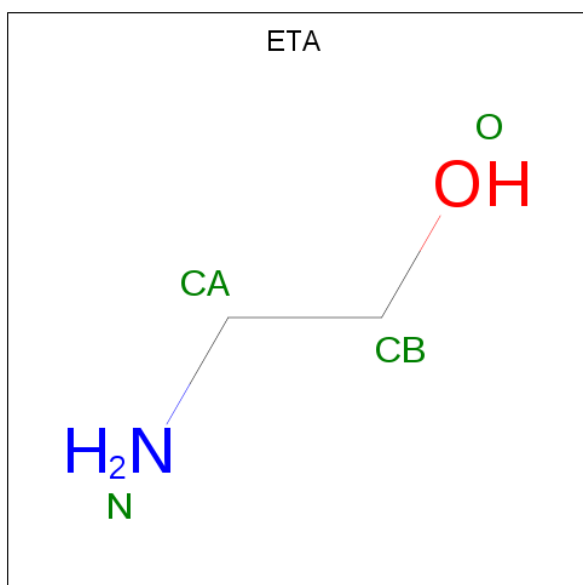
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			10	6	4		

- Molecule 4 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula:  $C_4H_{10}O_3$ ).



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

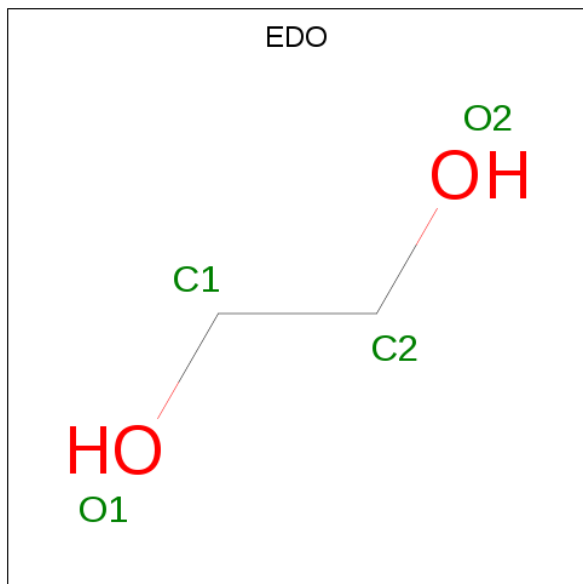
- Molecule 5 is ETHANOLAMINE (three-letter code: ETA) (formula:  $C_2H_7NO$ ).





Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			4	2	1	1		
5	B	1	Total	C	N	O	0	0
			4	2	1	1		
5	C	1	Total	C	N	O	0	0
			4	2	1	1		
5	D	1	Total	C	N	O	0	0
			4	2	1	1		
5	E	1	Total	C	N	O	0	0
			4	2	1	1		
5	F	1	Total	C	N	O	0	0
			4	2	1	1		

- Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula:  $C_2H_6O_2$ ).



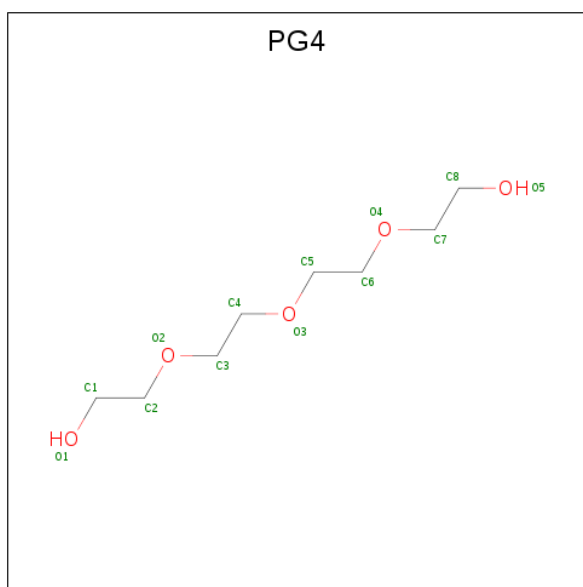
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			4	2	2		
6	B	1	Total	C	O	0	0
			4	2	2		
6	B	1	Total	C	O	0	0
			4	2	2		
6	B	1	Total	C	O	0	0
			4	2	2		
6	C	1	Total	C	O	0	0
			4	2	2		
6	C	1	Total	C	O	0	0
			4	2	2		
6	C	1	Total	C	O	0	0
			4	2	2		
6	C	1	Total	C	O	0	0
			4	2	2		
6	C	1	Total	C	O	0	0
			4	2	2		
6	D	1	Total	C	O	0	0
			4	2	2		
6	E	1	Total	C	O	0	0
			4	2	2		
6	E	1	Total	C	O	0	0
			4	2	2		
6	E	1	Total	C	O	0	0
			4	2	2		
6	E	1	Total	C	O	0	0
			4	2	2		
6	F	1	Total	C	O	0	0
			4	2	2		

- Molecule 7 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: C<sub>8</sub>H<sub>18</sub>O<sub>5</sub>).



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

- Molecule 8 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	D	1	Total	Mg	0	0
			1	1		
8	E	1	Total	Mg	0	0
			1	1		
8	B	1	Total	Mg	0	0
			1	1		
8	C	1	Total	Mg	0	0
			1	1		
8	A	1	Total	Mg	0	0
			1	1		

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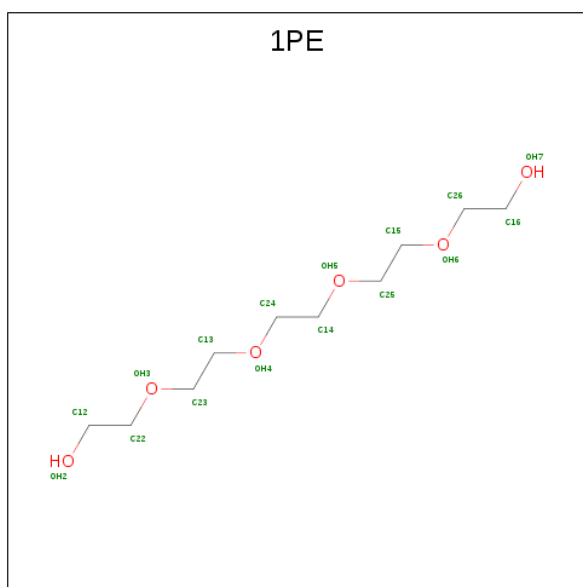
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	F	1	Total	Mg	0	0
			1	1		

- Molecule 9 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	B	1	Total	K	0	0
			1	1		
9	A	1	Total	K	0	0
			1	1		
9	D	1	Total	K	0	0
			1	1		

- Molecule 10 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: C<sub>10</sub>H<sub>22</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	C	1	Total	C	O	0	0
			16	10	6		
10	D	1	Total	C	O	0	0
			16	10	6		
10	E	1	Total	C	O	0	0
			16	10	6		

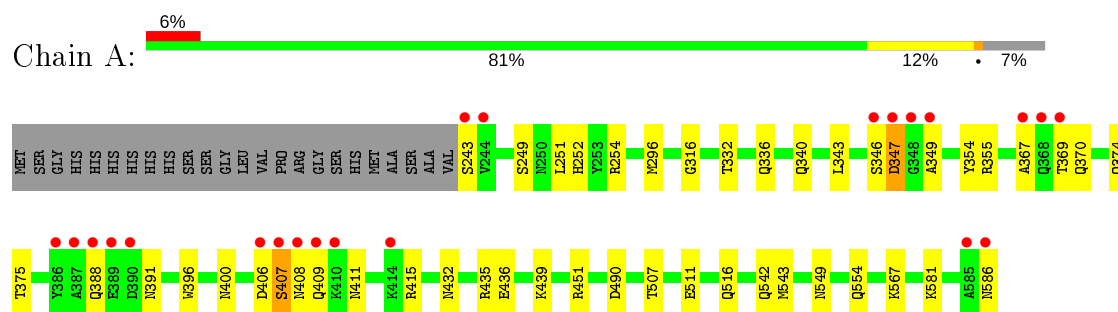
- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	195	Total 195	O 195	0	0
11	B	205	Total 205	O 205	0	0
11	C	201	Total 201	O 201	0	0
11	D	147	Total 147	O 147	0	0
11	E	133	Total 133	O 133	0	0
11	F	129	Total 129	O 129	0	0

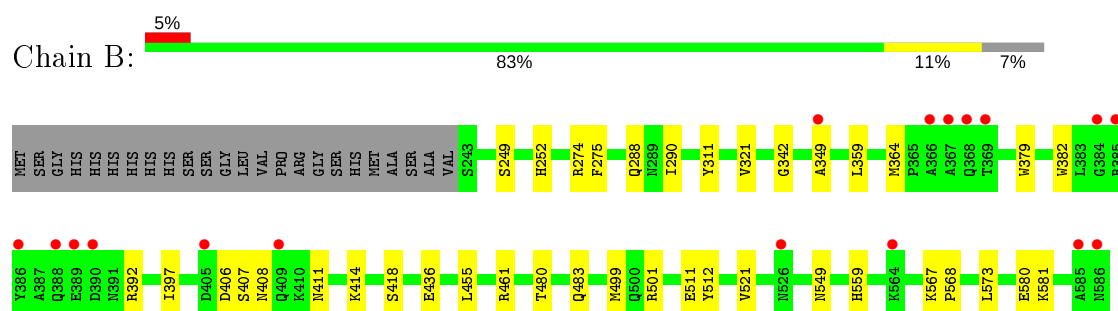
### 3 Residue-property plots [i](#)

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.

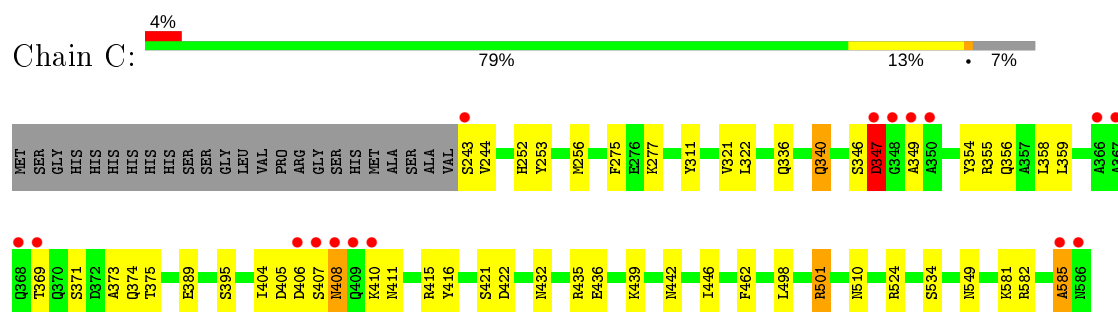
- Molecule 1: Periplasmic domain of the cardiolipin transporter protein YejM/PbgA



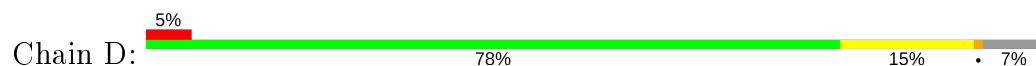
- Molecule 1: Periplasmic domain of the cardiolipin transporter protein YejM/PbgA

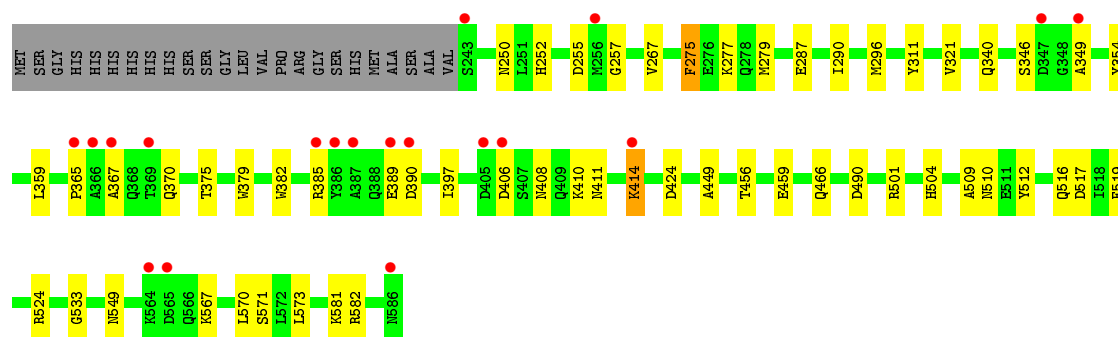


- Molecule 1: Periplasmic domain of the cardiolipin transporter protein YejM/PbgA

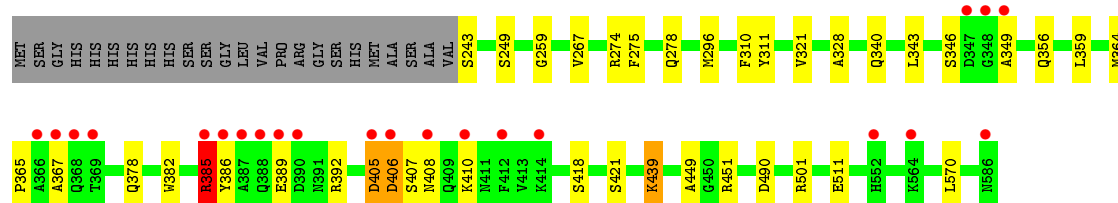
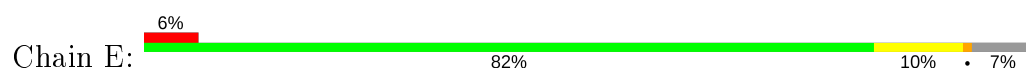


- Molecule 1: Periplasmic domain of the cardiolipin transporter protein YejM/PbgA

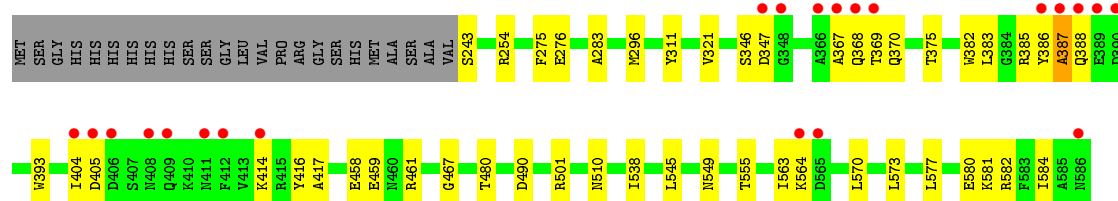
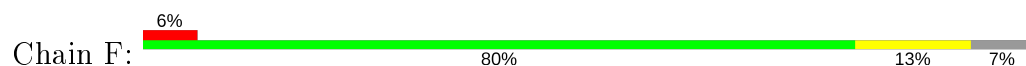




- Molecule 1: Periplasmic domain of the cardiolipin transporter protein YejM/PbgA



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



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	121.61Å 124.90Å 183.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.56 – 2.05 43.67 – 2.05	Depositor EDS
% Data completeness (in resolution range)	85.9 (43.56-2.05) 85.9 (43.67-2.05)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.09 (at 2.05Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, $R_{free}$	0.184 , 0.227 0.184 , 0.227	Depositor DCC
$R_{free}$ test set	7477 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	33.1	Xtriage
Anisotropy	0.212	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 49.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.009 for k,h,-l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	17703	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.32% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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, PGE, K, EDO, 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	0.35	0/2796	0.55	0/3809
1	B	0.35	0/2799	0.51	0/3813
1	C	0.32	0/2799	0.54	0/3813
1	D	0.31	0/2799	0.50	0/3813
1	E	0.31	0/2787	0.51	0/3797
1	F	0.30	0/2793	0.50	0/3805
All	All	0.32	0/16773	0.52	0/22850

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	2727	0	2637	36	0
1	B	2727	0	2639	27	0
1	C	2727	0	2638	41	0
1	D	2727	0	2639	39	0
1	E	2721	0	2629	27	0
1	F	2724	0	2634	33	0
2	A	19	0	26	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	19	0	26	3	0
2	C	19	0	26	1	0
3	A	10	0	14	0	0
3	B	10	0	14	0	0
4	A	7	0	10	0	0
5	A	4	0	7	1	0
5	B	4	0	7	0	0
5	C	4	0	7	0	0
5	D	4	0	7	0	0
5	E	4	0	7	1	0
5	F	4	0	7	0	0
6	A	24	0	36	3	0
6	B	16	0	24	3	0
6	C	20	0	30	5	0
6	D	4	0	6	1	0
6	E	16	0	24	4	0
6	F	4	0	6	0	0
7	A	13	0	18	2	0
7	B	13	0	18	3	0
7	D	13	0	18	4	0
7	E	13	0	18	3	0
7	F	39	0	54	7	0
8	A	1	0	0	0	0
8	B	1	0	0	0	0
8	C	1	0	0	0	0
8	D	1	0	0	0	0
8	E	1	0	0	0	0
8	F	1	0	0	0	0
9	A	1	0	0	0	0
9	B	1	0	0	0	0
9	D	1	0	0	0	0
10	C	16	0	22	4	0
10	D	16	0	22	2	0
10	E	16	0	22	0	0
11	A	195	0	0	6	0
11	B	205	0	0	2	0
11	C	201	0	0	5	0
11	D	147	0	0	3	0
11	E	133	0	0	1	0
11	F	129	0	0	3	0
All	All	17703	0	16292	199	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 6.

The worst 5 of 199 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:347:ASP:HB3	1:C:369:THR:HA	1.37	1.04
1:C:408:ASN:HB2	1:C:411:ASN:HB2	1.55	0.87
1:F:388:GLN:HE21	1:F:393:TRP:HE1	1.22	0.84
1:F:549:ASN:HA	7:F:605:PG4:H82	1.61	0.81
1:D:501:ARG:HD3	7:D:604:PG4:H51	1.62	0.80

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	344/368 (94%)	324 (94%)	16 (5%)	4 (1%)	13	5
1	B	345/368 (94%)	328 (95%)	17 (5%)	0	100	100
1	C	345/368 (94%)	323 (94%)	18 (5%)	4 (1%)	13	5
1	D	345/368 (94%)	331 (96%)	10 (3%)	4 (1%)	13	5
1	E	343/368 (93%)	326 (95%)	13 (4%)	4 (1%)	13	5
1	F	344/368 (94%)	323 (94%)	16 (5%)	5 (2%)	10	3
All	All	2066/2208 (94%)	1955 (95%)	90 (4%)	21 (1%)	15	6

5 of 21 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	367	ALA
1	A	407	SER
1	A	409	GLN
1	C	244	VAL
1	C	347	ASP

### 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	297/314 (95%)	296 (100%)	1 (0%)	92	93
1	B	298/314 (95%)	294 (99%)	4 (1%)	69	67
1	C	298/314 (95%)	291 (98%)	7 (2%)	50	44
1	D	298/314 (95%)	291 (98%)	7 (2%)	50	44
1	E	296/314 (94%)	289 (98%)	7 (2%)	49	42
1	F	297/314 (95%)	294 (99%)	3 (1%)	76	75
All	All	1784/1884 (95%)	1755 (98%)	29 (2%)	62	59

5 of 29 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	275	PHE
1	D	414	LYS
1	F	275	PHE
1	D	340	GLN
1	D	571[A]	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	C	408	ASN
1	C	549	ASN
1	E	542	GLN
1	C	391	ASN
1	E	586	ASN

### 5.3.3 RNA ⓘ

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 52 ligands modelled in this entry, 9 are monoatomic - leaving 43 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	$\# Z  > 2$
10	1PE	E	602	-	15,15,15	0.51	0	14,14,14	0.24	0
6	EDO	A	1807	-	3,3,3	0.46	0	2,2,2	0.37	0
7	PG4	E	607	-	12,12,12	0.51	0	11,11,11	0.28	0
6	EDO	F	602	-	3,3,3	0.49	0	2,2,2	0.26	0
5	ETA	D	601	-	3,3,3	0.44	0	2,2,2	0.56	0
2	P6G	A	1801	-	18,18,18	0.53	0	17,17,17	0.25	0
5	ETA	A	1804	-	3,3,3	0.54	0	2,2,2	0.65	0
6	EDO	C	1701	-	3,3,3	0.50	0	2,2,2	0.25	0
10	1PE	D	602	-	15,15,15	0.53	0	14,14,14	0.25	0
6	EDO	A	1806	-	3,3,3	0.56	0	2,2,2	0.23	0
6	EDO	B	604	-	3,3,3	0.45	0	2,2,2	0.42	0
6	EDO	A	1810	-	3,3,3	0.45	0	2,2,2	0.31	0
7	PG4	A	1811	-	12,12,12	0.53	0	11,11,11	0.41	0
6	EDO	E	606	-	3,3,3	0.51	0	2,2,2	0.18	0
6	EDO	E	603	-	3,3,3	0.46	0	2,2,2	0.35	0
6	EDO	C	1707	-	3,3,3	0.40	0	2,2,2	0.46	0
5	ETA	F	601	-	3,3,3	0.49	0	2,2,2	0.54	0
10	1PE	C	1708	-	15,15,15	0.53	0	14,14,14	0.28	0
6	EDO	C	1705	-	3,3,3	0.52	0	2,2,2	0.26	0
7	PG4	B	608	-	12,12,12	0.53	0	11,11,11	0.41	0
2	P6G	B	606	-	18,18,18	0.53	0	17,17,17	0.25	0
6	EDO	C	1704	-	3,3,3	0.49	0	2,2,2	0.26	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	ETA	B	601	-	3,3,3	0.48	0	2,2,2	0.94	0
7	PG4	D	604	-	12,12,12	0.52	0	11,11,11	0.32	0
6	EDO	B	605	-	3,3,3	0.47	0	2,2,2	0.26	0
5	ETA	E	601	-	3,3,3	0.34	0	2,2,2	0.76	0
7	PG4	F	605	-	12,12,12	0.50	0	11,11,11	0.32	0
2	P6G	C	1703	-	18,18,18	0.54	0	17,17,17	0.28	0
3	PGE	B	607	-	9,9,9	0.31	0	8,8,8	0.36	0
6	EDO	E	604	-	3,3,3	0.46	0	2,2,2	0.36	0
6	EDO	A	1809	-	3,3,3	0.42	0	2,2,2	0.40	0
6	EDO	D	603	-	3,3,3	0.51	0	2,2,2	0.10	0
6	EDO	E	605	-	3,3,3	0.46	0	2,2,2	0.36	0
5	ETA	C	1702	-	3,3,3	0.54	0	2,2,2	0.42	0
7	PG4	F	603	-	12,12,12	0.52	0	11,11,11	0.33	0
6	EDO	B	603	-	3,3,3	0.46	0	2,2,2	0.25	0
4	PEG	A	1803	-	6,6,6	0.47	0	5,5,5	0.34	0
7	PG4	F	604	-	12,12,12	0.51	0	11,11,11	0.23	0
6	EDO	B	602	-	3,3,3	0.46	0	2,2,2	0.31	0
3	PGE	A	1802	-	9,9,9	0.33	0	8,8,8	0.29	0
6	EDO	C	1706	-	3,3,3	0.41	0	2,2,2	0.45	0
6	EDO	A	1805	-	3,3,3	0.50	0	2,2,2	0.24	0
6	EDO	A	1808	-	3,3,3	0.41	0	2,2,2	0.39	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
10	1PE	E	602	-	-	10/13/13/13	-
6	EDO	A	1807	-	-	1/1/1/1	-
7	PG4	E	607	-	-	8/10/10/10	-
6	EDO	F	602	-	-	0/1/1/1	-
5	ETA	D	601	-	-	1/1/1/1	-
2	P6G	A	1801	-	-	13/16/16/16	-
5	ETA	A	1804	-	-	1/1/1/1	-
6	EDO	C	1701	-	-	1/1/1/1	-
10	1PE	D	602	-	-	6/13/13/13	-
6	EDO	A	1806	-	-	1/1/1/1	-
6	EDO	B	604	-	-	0/1/1/1	-
6	EDO	A	1810	-	-	1/1/1/1	-
7	PG4	A	1811	-	-	7/10/10/10	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	EDO	E	606	-	-	0/1/1/1	-
6	EDO	E	603	-	-	1/1/1/1	-
6	EDO	C	1707	-	-	1/1/1/1	-
5	ETA	F	601	-	-	1/1/1/1	-
10	1PE	C	1708	-	-	7/13/13/13	-
6	EDO	C	1705	-	-	0/1/1/1	-
7	PG4	B	608	-	-	4/10/10/10	-
2	P6G	B	606	-	-	3/16/16/16	-
6	EDO	C	1704	-	-	1/1/1/1	-
5	ETA	B	601	-	-	1/1/1/1	-
7	PG4	D	604	-	-	5/10/10/10	-
6	EDO	B	605	-	-	0/1/1/1	-
5	ETA	E	601	-	-	1/1/1/1	-
7	PG4	F	605	-	-	5/10/10/10	-
2	P6G	C	1703	-	-	7/16/16/16	-
3	PGE	B	607	-	-	4/7/7/7	-
6	EDO	E	604	-	-	0/1/1/1	-
6	EDO	A	1809	-	-	0/1/1/1	-
6	EDO	D	603	-	-	0/1/1/1	-
6	EDO	E	605	-	-	1/1/1/1	-
5	ETA	C	1702	-	-	1/1/1/1	-
7	PG4	F	603	-	-	5/10/10/10	-
6	EDO	B	603	-	-	0/1/1/1	-
4	PEG	A	1803	-	-	1/4/4/4	-
7	PG4	F	604	-	-	5/10/10/10	-
6	EDO	B	602	-	-	0/1/1/1	-
3	PGE	A	1802	-	-	4/7/7/7	-
6	EDO	C	1706	-	-	0/1/1/1	-
6	EDO	A	1805	-	-	0/1/1/1	-
6	EDO	A	1808	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 108 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	D	601	ETA	N-CA-CB-O
5	B	601	ETA	N-CA-CB-O

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Mol	Chain	Res	Type	Atoms
2	C	1703	P6G	C14-C15-O16-C17
7	A	1811	PG4	C4-C3-O2-C2
10	E	602	1PE	OH7-C16-C26-OH6

There are no ring outliers.

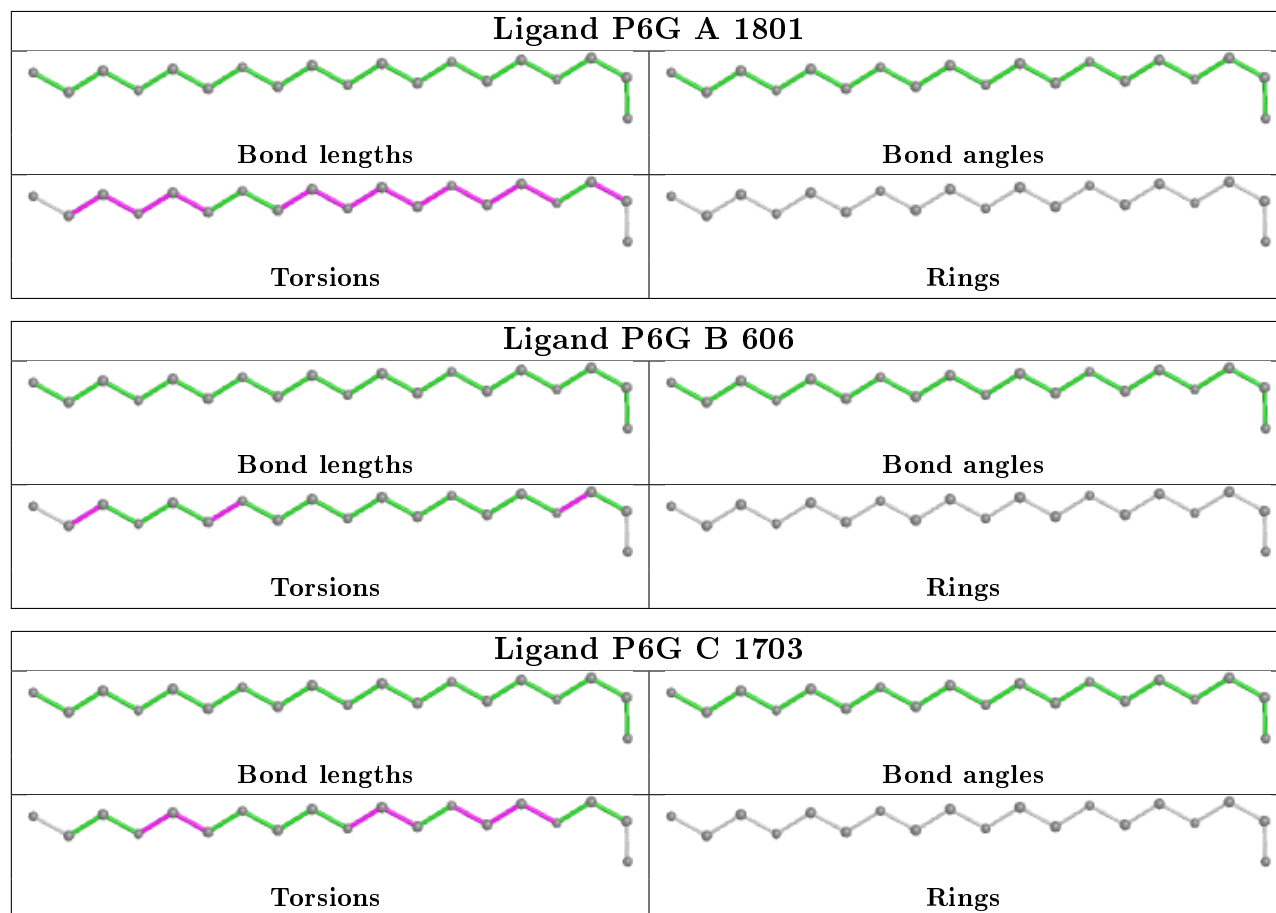
26 monomers are involved in 48 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	E	607	PG4	3	0
2	A	1801	P6G	1	0
5	A	1804	ETA	1	0
6	C	1701	EDO	1	0
10	D	602	1PE	2	0
6	B	604	EDO	2	0
6	A	1810	EDO	2	0
7	A	1811	PG4	2	0
6	E	603	EDO	2	0
10	C	1708	1PE	4	0
6	C	1705	EDO	2	0
7	B	608	PG4	3	0
2	B	606	P6G	3	0
6	C	1704	EDO	1	0
7	D	604	PG4	4	0
6	B	605	EDO	1	0
5	E	601	ETA	1	0
7	F	605	PG4	1	0
2	C	1703	P6G	1	0
6	E	604	EDO	2	0
6	A	1809	EDO	1	0
6	D	603	EDO	1	0
7	F	603	PG4	5	0
7	F	604	PG4	1	0
6	C	1706	EDO	1	0
6	A	1808	EDO	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	344/368 (93%)	-0.04	22 (6%) 19 21	19, 37, 93, 160	0
1	B	344/368 (93%)	0.09	17 (4%) 29 31	21, 36, 84, 140	0
1	C	344/368 (93%)	-0.03	16 (4%) 31 33	20, 37, 99, 167	0
1	D	344/368 (93%)	0.21	19 (5%) 25 27	26, 43, 98, 186	0
1	E	344/368 (93%)	0.16	22 (6%) 19 21	28, 47, 95, 180	0
1	F	344/368 (93%)	0.22	22 (6%) 19 21	27, 46, 108, 175	0
All	All	2064/2208 (93%)	0.10	118 (5%) 23 25	19, 41, 97, 186	0

The worst 5 of 118 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	386	TYR	22.2
1	F	386	TYR	15.4
1	E	386	TYR	13.8
1	C	586	ASN	12.1
1	F	387	ALA	12.0

### 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 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
6	EDO	F	602	4/4	0.28	0.23	85,86,87,88	0
6	EDO	A	1805	4/4	0.53	0.28	71,72,72,72	0
6	EDO	E	605	4/4	0.54	0.19	70,70,71,72	0
7	PG4	A	1811	13/13	0.59	0.20	70,73,81,81	0
6	EDO	C	1705	4/4	0.65	0.24	62,62,63,63	0
6	EDO	B	605	4/4	0.70	0.23	61,64,65,67	0
6	EDO	E	606	4/4	0.72	0.40	72,72,72,72	0
6	EDO	E	604	4/4	0.74	0.27	67,68,68,68	0
6	EDO	A	1810	4/4	0.75	0.27	58,60,63,67	0
4	PEG	A	1803	7/7	0.76	0.38	66,71,75,75	0
6	EDO	E	603	4/4	0.77	0.24	61,65,67,70	0
10	1PE	C	1708	16/16	0.77	0.21	68,74,78,80	0
6	EDO	D	603	4/4	0.78	0.27	64,67,68,69	0
6	EDO	A	1806	4/4	0.79	0.18	46,52,53,55	0
6	EDO	C	1704	4/4	0.79	0.17	57,61,65,67	0
3	PGE	A	1802	10/10	0.80	0.15	56,60,67,68	0
3	PGE	B	607	10/10	0.80	0.15	72,73,74,74	0
7	PG4	F	603	13/13	0.81	0.14	61,66,76,76	0
7	PG4	F	605	13/13	0.81	0.16	59,70,74,75	0
2	P6G	B	606	19/19	0.82	0.17	41,53,71,71	0
2	P6G	A	1801	19/19	0.83	0.14	54,62,75,75	0
6	EDO	B	602	4/4	0.83	0.44	71,72,72,72	0
2	P6G	C	1703	19/19	0.83	0.14	50,63,68,69	0
10	1PE	D	602	16/16	0.83	0.14	66,70,72,73	0
5	ETA	F	601	4/4	0.84	0.11	63,65,67,68	0
10	1PE	E	602	16/16	0.84	0.15	56,62,69,69	0
6	EDO	A	1807	4/4	0.85	0.30	60,61,63,63	0
6	EDO	B	604	4/4	0.86	0.30	44,51,52,54	0
6	EDO	C	1701	4/4	0.86	0.35	51,56,64,68	0
7	PG4	F	604	13/13	0.86	0.14	54,59,65,68	0
6	EDO	C	1707	4/4	0.87	0.21	44,46,50,53	0
7	PG4	E	607	13/13	0.88	0.16	60,61,64,65	0
6	EDO	B	603	4/4	0.89	0.28	44,53,62,70	0
7	PG4	B	608	13/13	0.89	0.12	46,48,63,63	0
5	ETA	E	601	4/4	0.89	0.14	36,39,41,47	0
7	PG4	D	604	13/13	0.91	0.12	52,57,73,73	0
6	EDO	A	1808	4/4	0.91	0.29	68,69,70,70	0

*Continued on next page...*

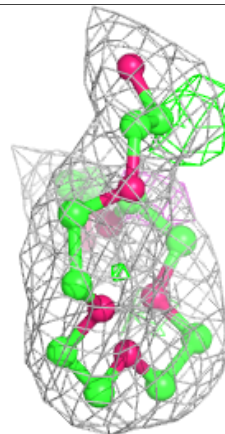
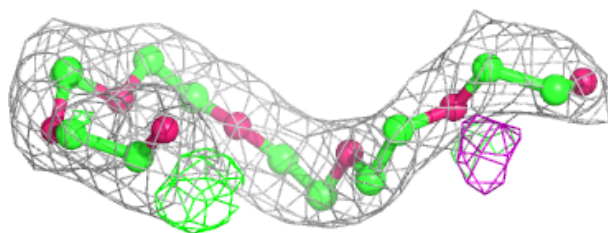
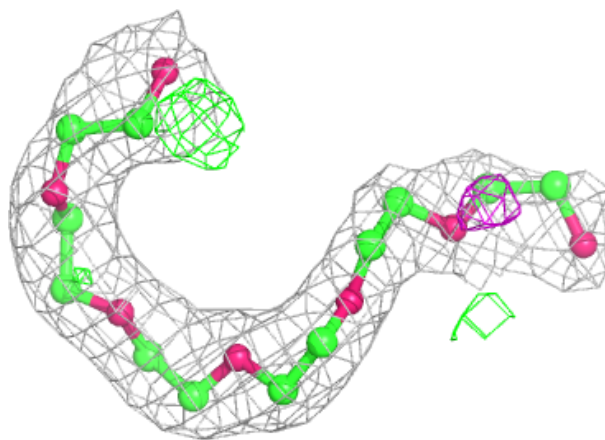
*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	ETA	B	601	4/4	0.92	0.15	39,43,45,46	0
5	ETA	A	1804	4/4	0.93	0.12	41,42,43,43	0
6	EDO	C	1706	4/4	0.94	0.14	41,43,43,45	0
5	ETA	D	601	4/4	0.94	0.14	45,45,47,48	0
6	EDO	A	1809	4/4	0.94	0.26	41,47,53,57	0
8	MG	D	605	1/1	0.95	0.14	43,43,43,43	0
8	MG	F	606	1/1	0.97	0.11	45,45,45,45	0
9	K	D	606	1/1	0.97	0.08	61,61,61,61	0
5	ETA	C	1702	4/4	0.97	0.08	29,32,32,33	0
8	MG	C	1709	1/1	0.97	0.14	33,33,33,33	0
9	K	B	610	1/1	0.98	0.08	56,56,56,56	0
8	MG	E	608	1/1	0.98	0.05	43,43,43,43	0
8	MG	A	1812	1/1	0.99	0.10	31,31,31,31	0
8	MG	B	609	1/1	0.99	0.14	33,33,33,33	0
9	K	A	1813	1/1	0.99	0.27	43,43,43,43	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.

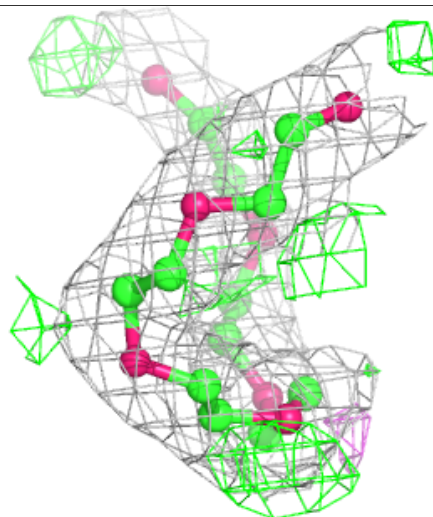
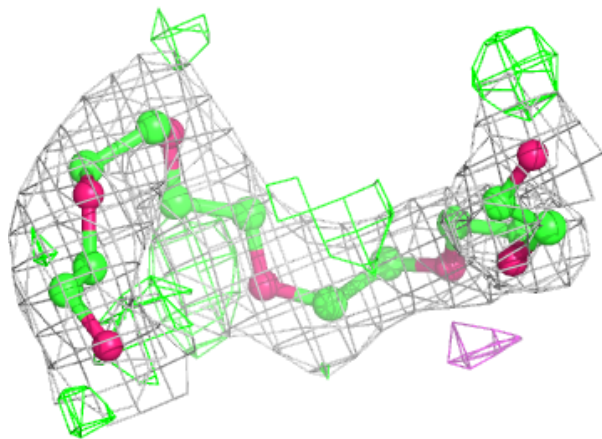
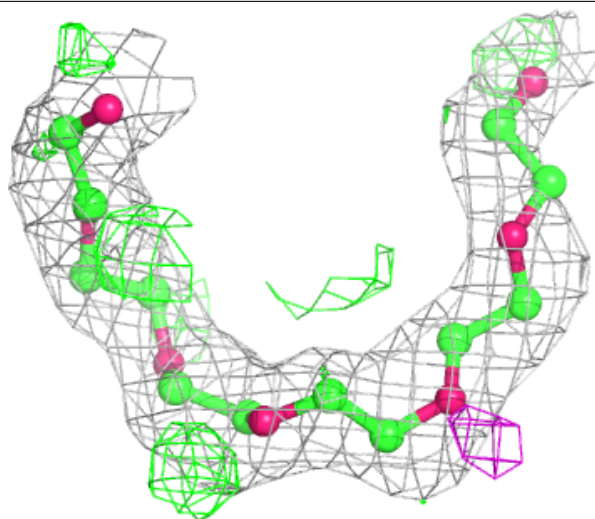
**Electron density around P6G B 606:**

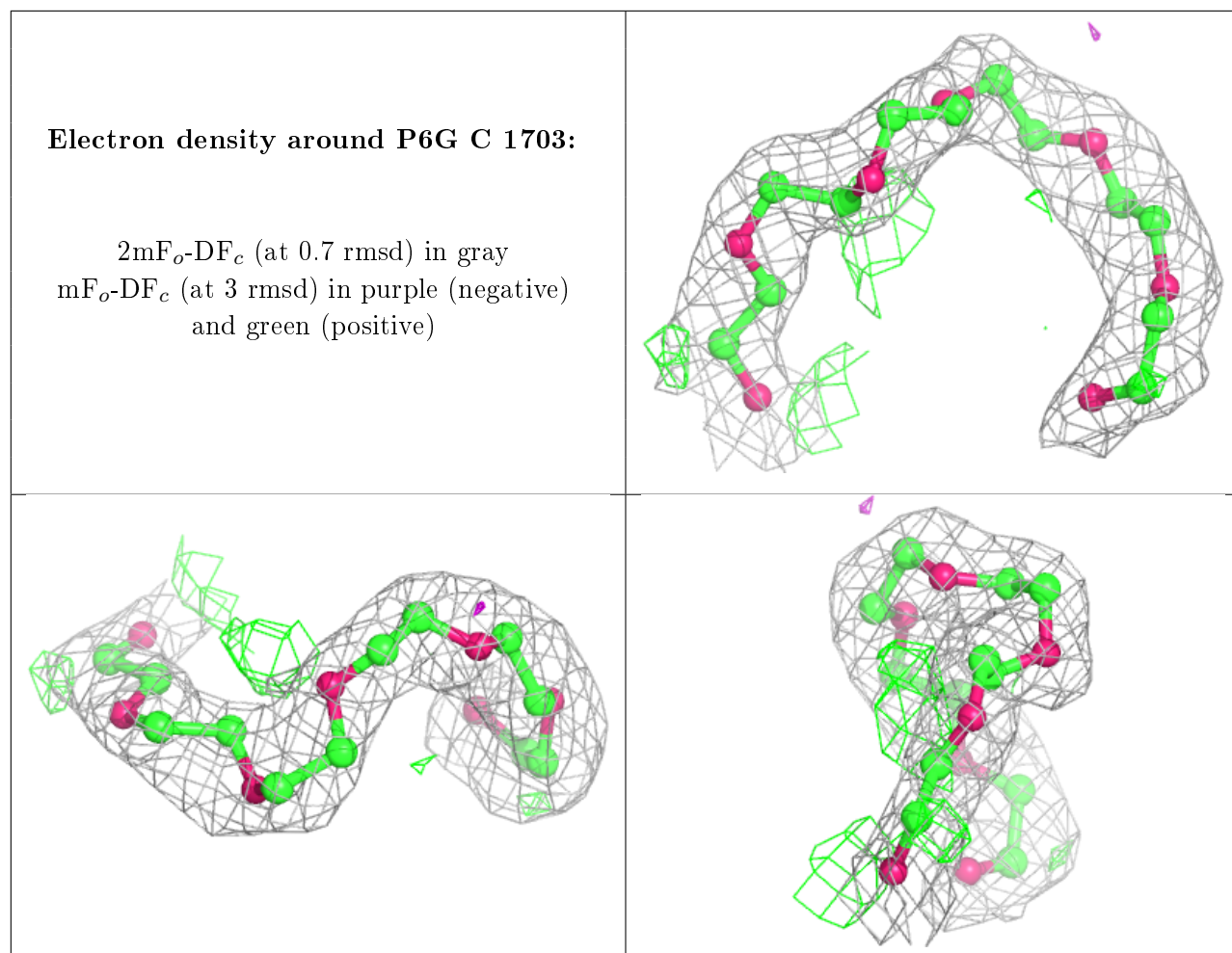
2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around P6G A 1801:**

$2mF_o-DF_c$  (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.