Full wwPDB X-ray Structure Validation Report ⓘ

Nov 7, 2023 – 05:12 AM EST

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

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

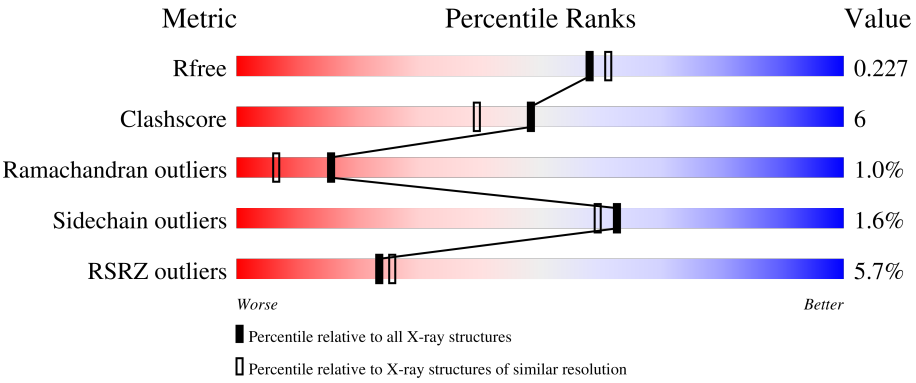
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.05 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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	368	6% 81% 12% • 7%
1	B	368	5% 83% 11% 7%
1	C	368	4% 79% 13% • 7%
1	D	368	5% 78% 15% • 7%
1	E	368	6% 83% 10% • 7%

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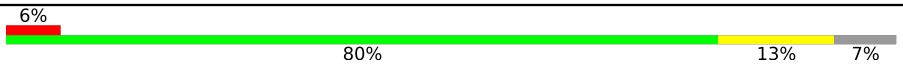
Mol	Chain	Length	Quality of chain
1	F	368	

2 Entry composition (i)

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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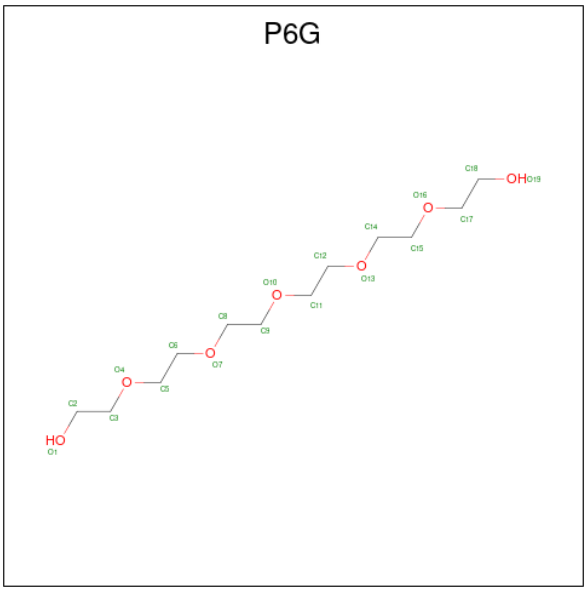
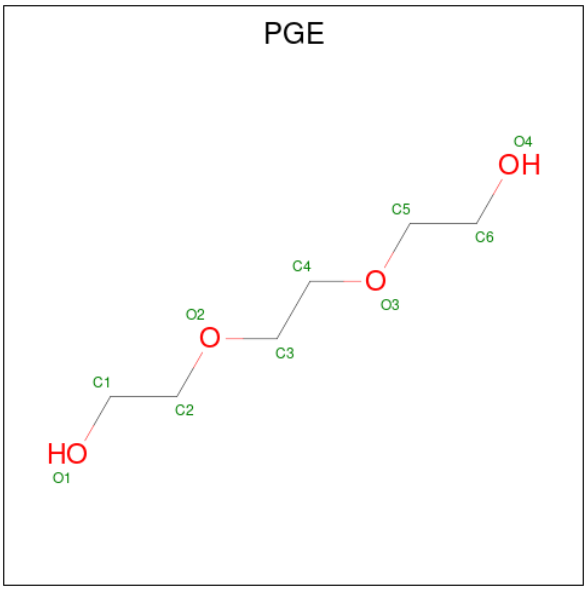
Chain	Residue	Modelled	Actual	Comment	Reference
E	227	HIS	-	expression tag	UNP A0A5A8TP41
E	228	SER	-	expression tag	UNP A0A5A8TP41
E	229	SER	-	expression tag	UNP A0A5A8TP41
E	230	GLY	-	expression tag	UNP A0A5A8TP41
E	231	LEU	-	expression tag	UNP A0A5A8TP41
E	232	VAL	-	expression tag	UNP A0A5A8TP41
E	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: $C_{12}H_{26}O_7$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 19 12 7	0	0
2	B	1	Total C O 19 12 7	0	0
2	C	1	Total C O 19 12 7	0	0

- Molecule 3 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



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

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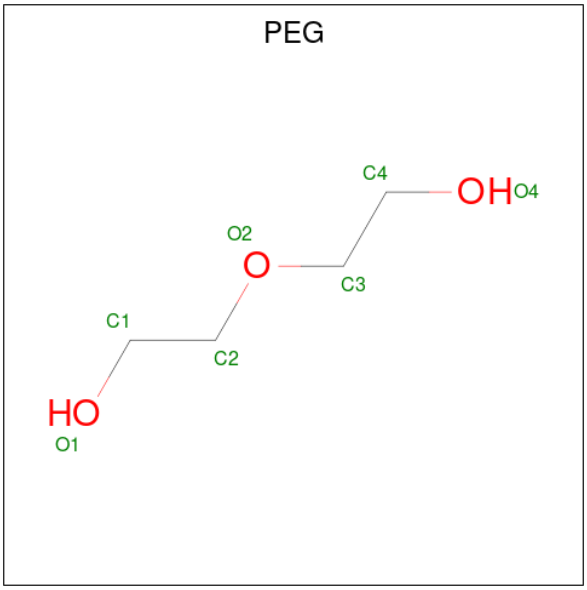
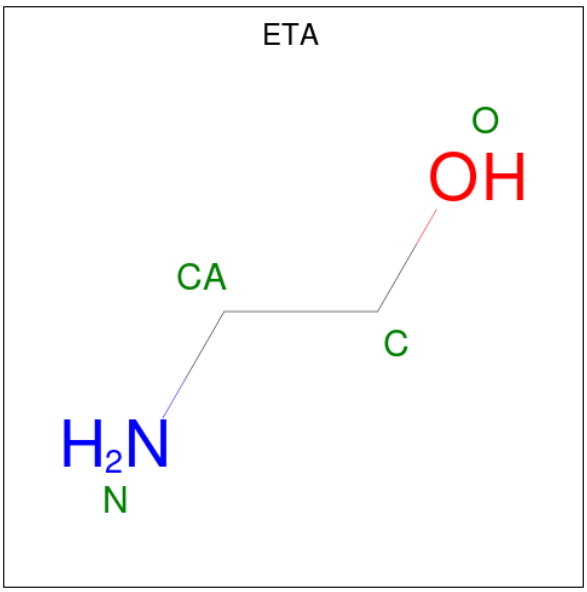
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total C O 10 6 4	0	0

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



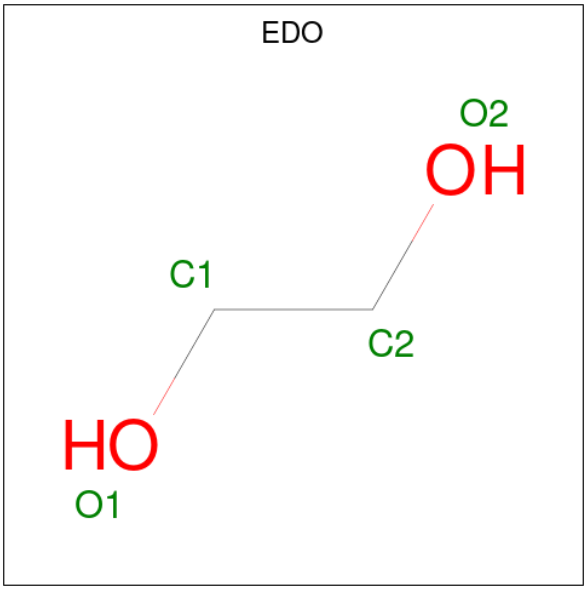
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 7 4 3	0	0

- 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 4 2 1 1	0	0
5	B	1	Total C N O 4 2 1 1	0	0
5	C	1	Total C N O 4 2 1 1	0	0
5	D	1	Total C N O 4 2 1 1	0	0
5	E	1	Total C N O 4 2 1 1	0	0
5	F	1	Total C N O 4 2 1 1	0	0

- 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 4 2 2	0	0
6	A	1	Total C O 4 2 2	0	0
6	A	1	Total C O 4 2 2	0	0
6	A	1	Total C O 4 2 2	0	0
6	A	1	Total C O 4 2 2	0	0
6	A	1	Total C O 4 2 2	0	0

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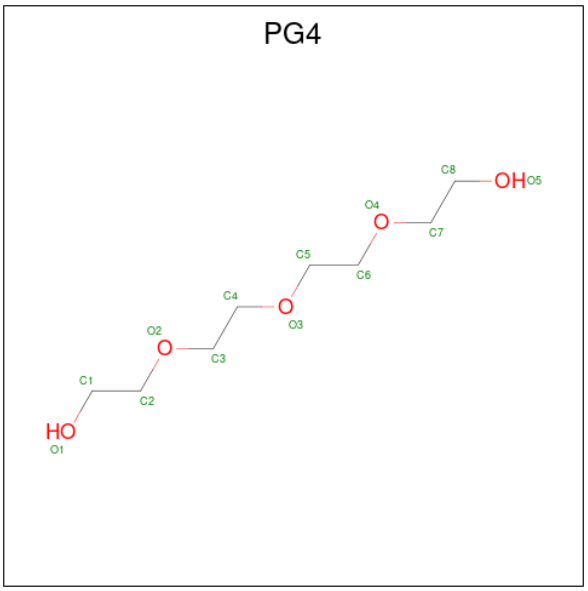
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			4	2	2		
6	B	1	Total	C	O	0	0
			4	2	2		
6	B	1	Total	C	O	0	0
			4	2	2		
6	B	1	Total	C	O	0	0
			4	2	2		
6	C	1	Total	C	O	0	0
			4	2	2		
6	C	1	Total	C	O	0	0
			4	2	2		
6	C	1	Total	C	O	0	0
			4	2	2		
6	C	1	Total	C	O	0	0
			4	2	2		
6	C	1	Total	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: $C_8H_{18}O_5$).



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

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

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

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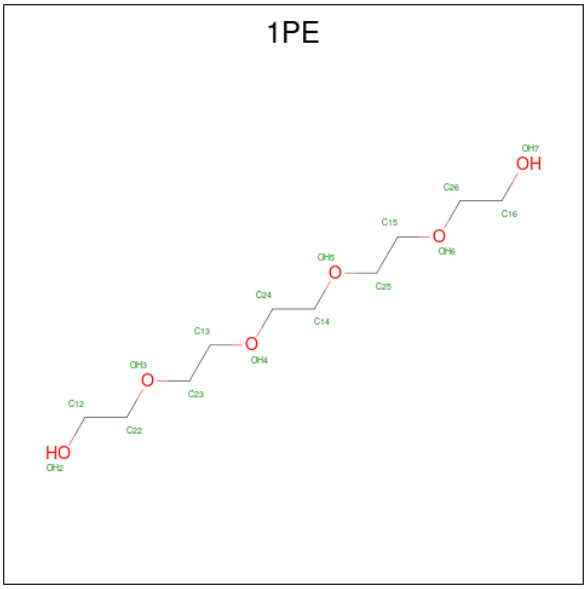
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	F	1	Total Mg 1 1	0	0

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

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

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



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

- Molecule 11 is water.

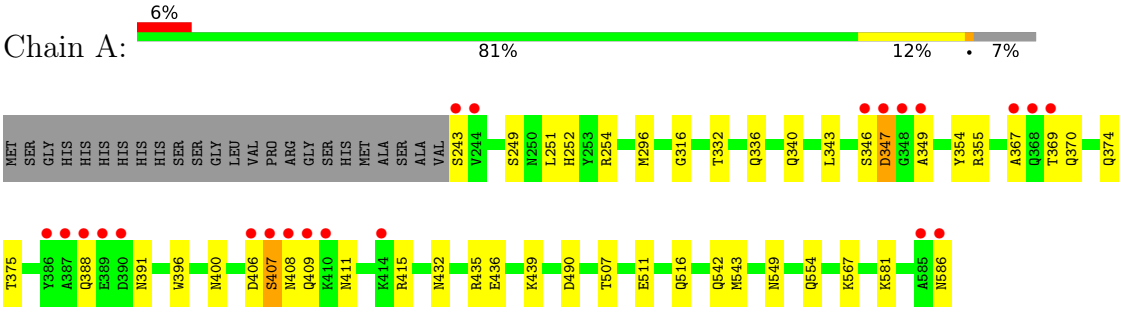
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	195	Total O 195 195	0	0
11	B	205	Total O 205 205	0	0
11	C	201	Total O 201 201	0	0
11	D	147	Total O 147 147	0	0
11	E	133	Total O 133 133	0	0
11	F	129	Total O 129 129	0	0

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.

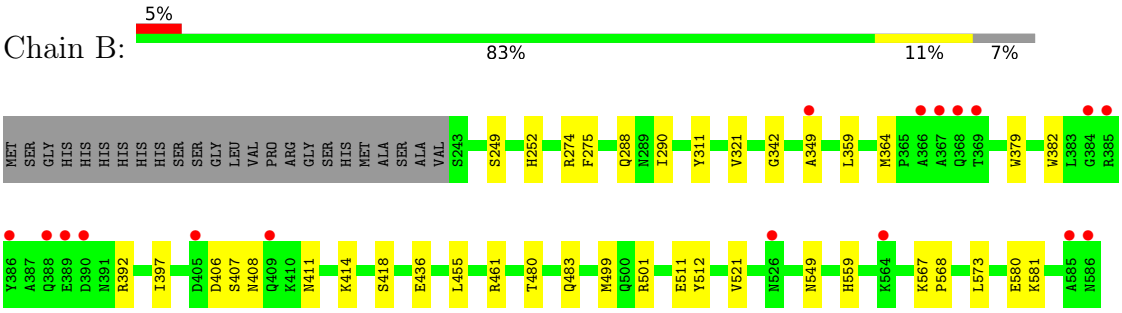
• Molecule 1: Periplasmic domain of the cardiolipin transporter protein YejM/PbgA

Chain A:



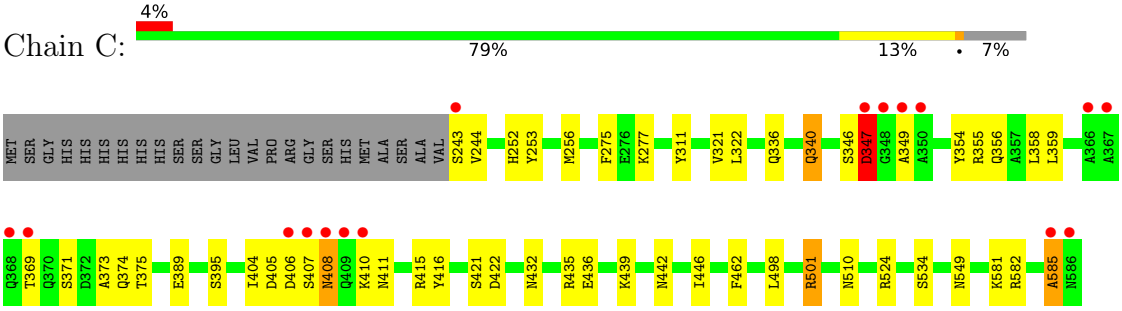
• Molecule 1: Periplasmic domain of the cardiolipin transporter protein YejM/PbgA

Chain B:



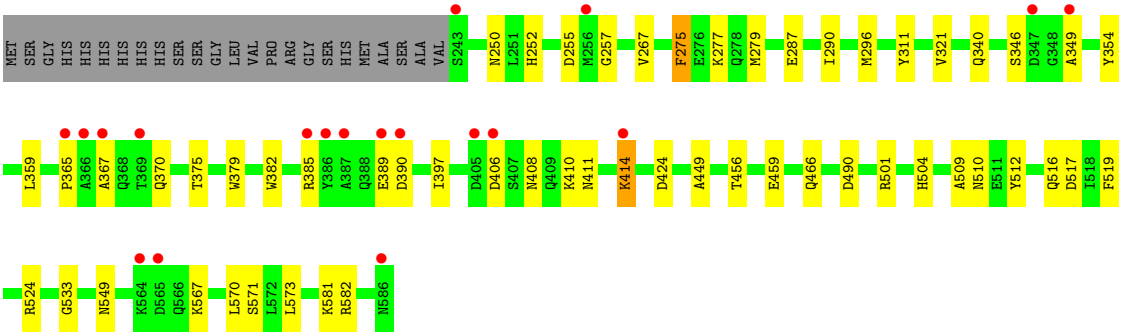
• Molecule 1: Periplasmic domain of the cardiolipin transporter protein YejM/PbgA

Chain C:

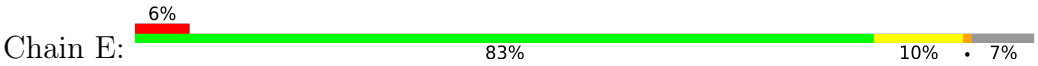


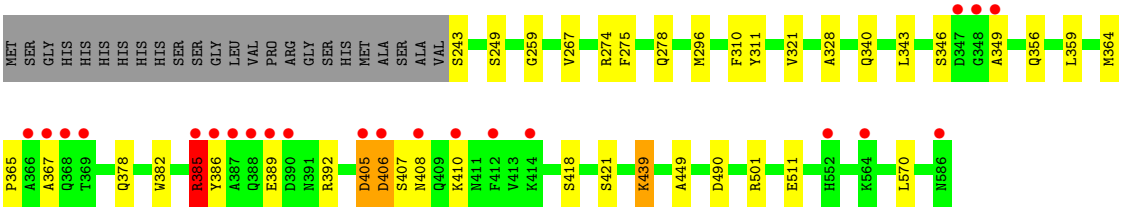
• Molecule 1: Periplasmic domain of the cardiolipin transporter protein YejM/PbgA

Chain D:

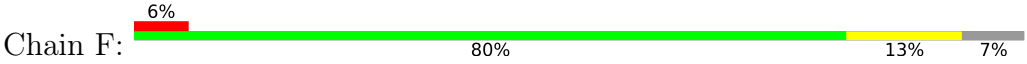


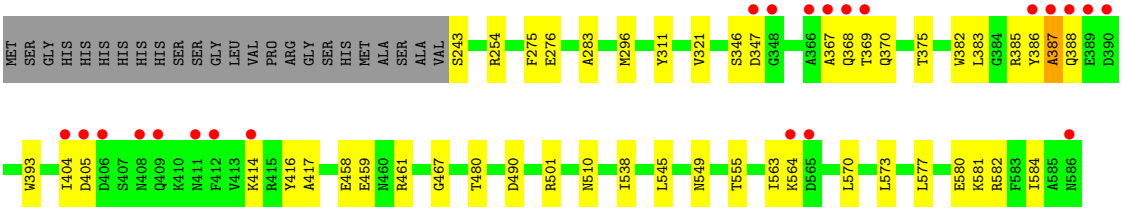
• Molecule 1: Periplasmic domain of the cardiolipin transporter protein YejM/PbgA





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





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	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
$< I/\sigma(I) >$ [1]	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^2)	33.1	Xtriage
Anisotropy	0.212	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 49.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	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^2)	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, PGE, 1PE, ETA, PEG, K, EDO, P6G, PG4

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

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	35	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	26	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	0	1	0
5	B	4	0	0	0	0
5	C	4	0	0	0	0
5	D	4	0	0	0	0
5	E	4	0	0	0	0
5	F	4	0	0	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	7	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	16250	198	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.

All (198) 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
1:E:382:TRP:O	1:E:385:ARG:HG3	1.81	0.80
1:C:349:ALA:HB1	1:C:359:LEU:HD11	1.66	0.77
1:A:254:ARG:NH2	11:A:1901:HOH:O	2.17	0.77
1:F:458:GLU:HA	1:F:461:ARG:HD2	1.67	0.76
1:D:349:ALA:HB1	1:D:359:LEU:HD21	1.70	0.74
1:A:347:ASP:OD1	1:A:400:ASN:ND2	2.21	0.74
1:C:408:ASN:HB2	1:C:411:ASN:CB	2.20	0.70
1:A:406:ASP:O	1:A:415:ARG:NH2	2.25	0.69
1:B:342:GLY:HA3	6:B:604:EDO:H22	1.73	0.69
1:D:549:ASN:HA	10:D:602:1PE:H162	1.75	0.69
1:F:254:ARG:NH2	11:F:701:HOH:O	2.25	0.69
1:F:501:ARG:HH11	7:F:603:PG4:H42	1.57	0.68
1:E:501:ARG:HH22	7:E:607:PG4:H11	1.57	0.68
1:C:407:SER:O	1:C:408:ASN:ND2	2.28	0.67
1:A:542:GLN:NE2	11:A:1903:HOH:O	2.28	0.67
6:C:1704:EDO:H22	1:D:277:LYS:HG3	1.77	0.67
1:E:501:ARG:HH11	7:E:607:PG4:H72	1.60	0.67
1:A:581:LYS:HG3	7:A:1811:PG4:H82	1.75	0.67
1:A:346:SER:HA	1:A:375:THR:OG1	1.95	0.67
1:D:466:GLN:OE1	11:D:702:HOH:O	2.12	0.67
1:D:287:GLU:OE2	11:D:701:HOH:O	2.12	0.66
1:E:274:ARG:HD3	6:E:604:EDO:H11	1.75	0.66
1:A:252:HIS:H	1:A:507:THR:CG2	2.10	0.65
1:B:288:GLN:OE1	11:B:701:HOH:O	2.15	0.64
1:D:456:THR:HG23	1:D:459:GLU:H	1.63	0.64
1:B:480:THR:HG21	2:B:606:P6G:H141	1.79	0.63
1:D:501:ARG:NH1	7:D:604:PG4:H82	2.14	0.63
1:A:432:ASN:O	1:A:436:GLU:HG2	1.98	0.62
1:C:534:SER:HA	1:C:549:ASN:HD22	1.64	0.62
1:F:555:THR:HG22	1:F:563:ILE:HD12	1.82	0.62
1:C:347:ASP:CB	1:C:369:THR:HA	2.24	0.60
1:B:461:ARG:NH2	1:B:559:HIS:O	2.34	0.59
1:C:462:PHE:HB2	6:C:1706:EDO:H21	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:501:ARG:HH22	10:C:1708:1PE:H161	1.67	0.59
7:A:1811:PG4:H12	1:C:581:LYS:HG3	1.85	0.58
1:A:516:GLN:HE21	6:A:1810:EDO:H12	1.69	0.58
1:F:370:GLN:HB3	11:F:703:HOH:O	2.04	0.57
1:E:392:ARG:HH21	6:E:603:EDO:H11	1.70	0.57
1:F:385:ARG:HH22	1:F:388:GLN:HB2	1.70	0.57
1:F:581:LYS:HB3	1:F:584:ILE:HD12	1.86	0.57
1:D:408:ASN:HD22	1:D:411:ASN:H	1.52	0.56
1:A:340:GLN:OE1	11:A:1902:HOH:O	2.17	0.56
1:E:259:GLY:HA3	6:E:603:EDO:H12	1.86	0.56
1:F:480:THR:HG21	7:F:603:PG4:H22	1.87	0.56
1:C:243:SER:HA	1:C:585:ALA:O	2.07	0.55
1:C:355:ARG:O	11:C:1801:HOH:O	2.17	0.55
1:A:349:ALA:HA	1:A:354:TYR:CG	2.43	0.54
1:F:347:ASP:OD1	1:F:369:THR:HG23	2.07	0.54
1:B:499:MET:HG3	1:B:512:TYR:CE1	2.42	0.54
1:C:581:LYS:HZ2	2:C:1703:P6G:H61	1.72	0.54
1:D:501:ARG:HH11	7:D:604:PG4:H82	1.72	0.54
1:D:516:GLN:HB2	1:D:524:ARG:HE	1.73	0.54
1:D:389:GLU:H	1:D:389:GLU:CD	2.10	0.53
1:D:390:ASP:N	1:D:390:ASP:OD1	2.40	0.53
1:A:554:GLN:HB2	6:A:1808:EDO:H11	1.90	0.53
1:A:567:LYS:HG2	6:C:1701:EDO:H11	1.89	0.53
1:F:311:TYR:CE2	1:F:321:VAL:HG11	2.43	0.53
1:C:404:ILE:HD12	1:C:416:TYR:HA	1.91	0.53
1:D:311:TYR:CE2	1:D:321:VAL:HG11	2.44	0.53
1:D:250:ASN:ND2	11:D:706:HOH:O	2.41	0.52
5:A:1804:ETA:N	11:A:1904:HOH:O	2.33	0.52
1:B:573:LEU:HD13	1:E:570:LEU:HD22	1.90	0.52
1:B:311:TYR:CE2	1:B:321:VAL:HG11	2.45	0.52
1:C:421[B]:SER:OG	11:C:1802:HOH:O	2.19	0.52
1:C:510:ASN:O	1:C:582:ARG:NH1	2.42	0.52
1:D:257:GLY:HA2	1:D:504:HIS:CG	2.45	0.51
1:D:275:PHE:HB2	1:D:279:MET:HE3	1.91	0.51
1:F:404:ILE:CD1	1:F:416:TYR:HA	2.40	0.51
1:B:274:ARG:HD2	1:B:455:LEU:HD12	1.92	0.51
1:A:347:ASP:HA	1:A:369:THR:HA	1.93	0.51
1:C:501:ARG:HD3	10:C:1708:1PE:H142	1.92	0.51
1:F:501:ARG:HG2	7:F:603:PG4:H72	1.93	0.51
1:A:549:ASN:OD1	1:A:549:ASN:N	2.44	0.51
1:B:408:ASN:ND2	1:B:411:ASN:HB2	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:382:TRP:O	1:D:385:ARG:HG2	2.11	0.51
1:A:391:ASN:OD1	1:A:391:ASN:N	2.44	0.50
1:A:388:GLN:O	1:A:388:GLN:HG2	2.11	0.50
1:D:275:PHE:HB2	1:D:279:MET:CE	2.42	0.50
1:D:370:GLN:NE2	1:D:375:THR:OG1	2.44	0.50
1:D:379:TRP:CG	1:D:397:ILE:HD11	2.47	0.49
1:C:349:ALA:HA	1:C:354:TYR:CB	2.43	0.49
1:E:349:ALA:HB1	1:E:359:LEU:HD11	1.95	0.49
1:A:316:GLY:HA3	2:A:1801:P6G:H52	1.93	0.49
1:C:501:ARG:HG3	10:C:1708:1PE:H121	1.95	0.49
1:E:343:LEU:HD23	1:E:359:LEU:HD21	1.95	0.49
1:E:405:ASP:OD2	1:E:406:ASP:N	2.46	0.49
1:B:436:GLU:O	6:B:605:EDO:H12	2.13	0.49
1:F:276:GLU:HA	1:F:283:ALA:HB2	1.95	0.49
1:B:290:ILE:HG12	1:B:483:GLN:HG2	1.95	0.48
1:B:406:ASP:OD2	1:B:411:ASN:HB3	2.13	0.48
1:F:538:ILE:HD12	1:F:545:LEU:HD22	1.95	0.48
1:C:446:ILE:HD11	1:C:498:LEU:HD21	1.96	0.48
1:A:567:LYS:NZ	11:A:1913:HOH:O	2.47	0.48
1:B:501:ARG:HH12	2:B:606:P6G:H181	1.79	0.48
1:C:524:ARG:NH1	11:C:1815:HOH:O	2.47	0.48
1:E:501:ARG:NH1	7:E:607:PG4:H72	2.29	0.48
1:C:346:SER:HA	1:C:375:THR:OG1	2.14	0.47
1:C:435:ARG:HD3	11:C:1878:HOH:O	2.13	0.47
1:D:570:LEU:HD22	1:F:573:LEU:HD13	1.95	0.47
1:E:278:GLN:HE21	6:E:604:EDO:H22	1.79	0.47
1:A:407:SER:HB3	1:A:415:ARG:HD3	1.96	0.47
1:D:501:ARG:HH12	7:D:604:PG4:H22	1.80	0.47
1:A:370:GLN:HB2	1:A:374:GLN:OE1	2.15	0.47
1:D:581:LYS:HD3	10:D:602:1PE:H132	1.97	0.47
1:F:501:ARG:HG2	7:F:603:PG4:H62	1.96	0.47
1:D:414:LYS:O	1:D:414:LYS:HE3	2.15	0.47
1:F:296:MET:O	1:F:490:ASP:HA	2.15	0.47
1:C:311:TYR:CE2	1:C:321:VAL:HG11	2.50	0.46
1:D:408:ASN:HD21	1:D:410:LYS:HB3	1.80	0.46
1:A:439:LYS:NZ	11:A:1915:HOH:O	2.48	0.46
1:E:311:TYR:CE2	1:E:321:VAL:HG11	2.50	0.46
1:D:408:ASN:ND2	1:D:410:LYS:HB3	2.30	0.46
1:C:442:ASN:O	11:C:1803:HOH:O	2.20	0.46
1:E:359:LEU:HD21	1:E:364:MET:HE2	1.98	0.46
1:C:406:ASP:OD1	1:C:415:ARG:HD3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:533:GLY:H	6:D:603:EDO:H22	1.80	0.46
1:F:414:LYS:HA	1:F:417:ALA:HB3	1.98	0.46
1:A:346:SER:O	1:A:370:GLN:HG2	2.15	0.46
1:D:279:MET:HG2	1:D:424:ASP:HB2	1.97	0.46
1:B:567:LYS:HG2	1:B:568:PRO:HD2	1.97	0.46
1:E:385:ARG:HH11	1:E:385:ARG:HB3	1.81	0.46
1:A:332:THR:O	1:A:336[B]:GLN:HG3	2.16	0.46
1:C:373:ALA:HB2	6:C:1705:EDO:H11	1.98	0.46
1:A:408:ASN:N	1:A:408:ASN:HD22	2.13	0.45
1:A:343:LEU:HD13	1:A:396:TRP:CE3	2.52	0.45
1:F:459:GLU:HB3	1:F:467:GLY:HA3	1.98	0.45
1:E:340:GLN:NE2	11:E:710:HOH:O	2.50	0.45
1:B:521:VAL:HG12	11:B:905:HOH:O	2.17	0.45
1:E:407:SER:OG	1:E:408:ASN:N	2.50	0.45
1:F:385:ARG:NH2	1:F:387:ALA:O	2.49	0.44
1:F:501:ARG:NH1	7:F:603:PG4:H42	2.28	0.44
1:A:407:SER:HB2	1:A:411:ASN:HB3	2.00	0.44
1:F:243:SER:N	11:F:716:HOH:O	2.49	0.44
1:C:256:MET:SD	1:E:356:GLN:HG2	2.58	0.44
1:B:349:ALA:HB2	1:B:364:MET:SD	2.58	0.44
1:C:422:ASP:HB3	6:C:1705:EDO:H21	2.00	0.44
1:F:577:LEU:O	1:F:581:LYS:HG2	2.17	0.44
1:B:379:TRP:CG	1:B:397:ILE:HD11	2.53	0.44
1:F:510:ASN:O	1:F:582:ARG:NH1	2.48	0.44
1:A:249:SER:OG	1:A:511:GLU:OE1	2.24	0.44
1:A:251:LEU:HA	1:A:507:THR:HG21	1.99	0.44
1:B:581:LYS:HZ2	7:B:608:PG4:H21	1.83	0.44
1:F:382:TRP:O	1:F:385:ARG:HD3	2.18	0.43
1:E:296:MET:O	1:E:490:ASP:HA	2.17	0.43
1:A:355:ARG:HH22	1:B:392:ARG:NH2	2.16	0.43
1:D:567:LYS:N	1:D:567:LYS:HD3	2.34	0.43
1:A:347:ASP:CG	1:A:400:ASN:HD21	2.21	0.43
1:B:249:SER:OG	1:B:511:GLU:OE1	2.25	0.43
1:D:573:LEU:HD13	1:F:570:LEU:HD22	2.01	0.43
6:A:1809:EDO:H11	6:A:1810:EDO:H21	2.01	0.43
1:F:346:SER:O	1:F:370:GLN:HG2	2.19	0.43
1:E:389:GLU:HG3	1:E:439:LYS:NZ	2.34	0.42
1:A:388:GLN:HA	1:A:439:LYS:HZ3	1.84	0.42
1:B:382:TRP:CE2	6:B:604:EDO:H21	2.54	0.42
1:B:414:LYS:HA	1:B:414:LYS:HD2	1.77	0.42
1:E:249:SER:OG	1:E:511:GLU:OE1	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:349:ALA:HB1	1:B:359:LEU:HD11	2.01	0.42
1:C:408:ASN:HB3	1:C:410:LYS:HE2	2.02	0.42
1:E:267:VAL:O	1:E:449:ALA:HA	2.20	0.42
1:E:364:MET:HG2	1:E:365:PRO:HD2	2.01	0.42
1:F:346:SER:HA	1:F:375:THR:OG1	2.19	0.42
1:C:253:TYR:CE2	1:C:336:GLN:HG2	2.54	0.42
1:E:310:PHE:O	1:E:328:ALA:HB1	2.20	0.42
1:C:354:TYR:HA	1:C:358:LEU:HB2	2.00	0.42
1:C:277:LYS:N	1:C:277:LYS:HD2	2.34	0.42
1:D:510:ASN:O	1:D:582:ARG:NH1	2.51	0.42
1:E:410:LYS:HB2	1:E:410:LYS:HE2	1.79	0.42
1:F:385:ARG:NH1	1:F:385:ARG:HB2	2.35	0.42
1:D:509:ALA:HA	1:D:512:TYR:CE2	2.55	0.42
1:D:501:ARG:NE	1:D:517:ASP:OD2	2.48	0.42
1:A:243:SER:O	1:A:586:ASN:HB2	2.20	0.41
1:B:549:ASN:HA	7:B:608:PG4:H82	2.02	0.41
1:C:407:SER:O	1:C:408:ASN:CG	2.59	0.41
1:A:435:ARG:NH2	11:A:1921:HOH:O	2.53	0.41
1:C:322:LEU:HB3	1:C:356:GLN:OE1	2.21	0.41
1:D:296:MET:O	1:D:490:ASP:HA	2.19	0.41
1:C:432:ASN:O	1:C:436:GLU:HG2	2.21	0.41
1:B:408:ASN:HD22	1:B:411:ASN:HB2	1.85	0.41
1:C:340:GLN:HE21	1:C:340:GLN:HB3	1.76	0.41
1:C:354:TYR:O	1:C:359:LEU:HB2	2.21	0.41
1:D:290:ILE:HD13	1:D:519:PHE:CE1	2.56	0.41
1:B:480:THR:CG2	2:B:606:P6G:H141	2.48	0.41
1:C:371:SER:OG	1:C:374:GLN:HG3	2.20	0.41
1:C:389:GLU:HG3	1:C:439:LYS:NZ	2.36	0.41
1:D:516:GLN:HB2	1:D:524:ARG:NE	2.36	0.41
1:A:296:MET:O	1:A:490:ASP:HA	2.21	0.41
1:B:580:GLU:HB3	7:B:608:PG4:H32	2.02	0.41
1:C:501:ARG:HH11	10:C:1708:1PE:H142	1.86	0.41
1:D:267:VAL:O	1:D:449:ALA:HA	2.21	0.41
1:F:580:GLU:HG3	7:F:604:PG4:H42	2.02	0.41
1:E:367:ALA:HB2	1:E:378:GLN:HE22	1.86	0.41
1:D:354:TYR:HB3	1:D:359:LEU:HD13	2.03	0.40
1:F:388:GLN:NE2	1:F:393:TRP:HE1	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	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

All (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
1	C	408	ASN
1	E	385	ARG
1	E	405	ASP
1	C	585	ALA
1	D	367	ALA
1	F	367	ALA
1	A	347	ASP
1	D	346	SER
1	E	346	SER
1	F	405	ASP
1	D	255	ASP
1	D	365	PRO
1	F	387	ALA
1	E	406	ASP
1	F	368	GLN

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Mol	Chain	Res	Type
1	F	386	TYR

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	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

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	543	MET
1	B	252	HIS
1	B	275	PHE
1	B	407	SER
1	B	418	SER
1	C	252	HIS
1	C	275	PHE
1	C	340	GLN
1	C	347	ASP
1	C	395	SER
1	C	405	ASP
1	C	501	ARG
1	D	252	HIS
1	D	275	PHE
1	D	340	GLN
1	D	406	ASP
1	D	414	LYS

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Mol	Chain	Res	Type
1	D	571[A]	SER
1	D	571[B]	SER
1	E	243	SER
1	E	275	PHE
1	E	385	ARG
1	E	386	TYR
1	E	418	SER
1	E	421	SER
1	E	439	LYS
1	F	275	PHE
1	F	383	LEU
1	F	564	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	408	ASN
1	A	460	ASN
1	B	466	GLN
1	B	552	HIS
1	C	340	GLN
1	C	388	GLN
1	C	391	ASN
1	C	408	ASN
1	C	549	ASN
1	D	340	GLN
1	D	370	GLN
1	D	408	ASN
1	E	378	GLN
1	E	542	GLN
1	E	586	ASN
1	F	340	GLN
1	F	388	GLN

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	$\#\|Z\| > 2$
6	EDO	C	1706	-	3,3,3	0.41	0	2,2,2	0.45	0
6	EDO	B	603	-	3,3,3	0.46	0	2,2,2	0.25	0
2	P6G	A	1801	-	18,18,18	0.53	0	17,17,17	0.25	0
6	EDO	E	605	-	3,3,3	0.46	0	2,2,2	0.36	0
6	EDO	A	1807	-	3,3,3	0.46	0	2,2,2	0.37	0
6	EDO	C	1707	-	3,3,3	0.40	0	2,2,2	0.46	0
6	EDO	A	1809	-	3,3,3	0.42	0	2,2,2	0.40	0
6	EDO	A	1806	-	3,3,3	0.56	0	2,2,2	0.23	0
7	PG4	F	604	-	12,12,12	0.51	0	11,11,11	0.23	0
5	ETA	F	601	-	3,3,3	0.49	0	2,2,2	0.54	0
5	ETA	A	1804	-	3,3,3	0.54	0	2,2,2	0.65	0
6	EDO	E	603	-	3,3,3	0.46	0	2,2,2	0.35	0
7	PG4	D	604	-	12,12,12	0.52	0	11,11,11	0.32	0
7	PG4	F	605	-	12,12,12	0.50	0	11,11,11	0.32	0
7	PG4	E	607	-	12,12,12	0.51	0	11,11,11	0.28	0
6	EDO	E	604	-	3,3,3	0.46	0	2,2,2	0.36	0
10	1PE	D	602	-	15,15,15	0.53	0	14,14,14	0.25	0
2	P6G	C	1703	-	18,18,18	0.54	0	17,17,17	0.28	0
7	PG4	B	608	-	12,12,12	0.53	0	11,11,11	0.41	0
6	EDO	B	604	-	3,3,3	0.45	0	2,2,2	0.42	0
5	ETA	C	1702	-	3,3,3	0.54	0	2,2,2	0.42	0
6	EDO	E	606	-	3,3,3	0.51	0	2,2,2	0.18	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	EDO	B	602	-	3,3,3	0.46	0	2,2,2	0.31	0
5	ETA	E	601	-	3,3,3	0.34	0	2,2,2	0.76	0
3	PGE	B	607	-	9,9,9	0.31	0	8,8,8	0.36	0
6	EDO	C	1701	-	3,3,3	0.50	0	2,2,2	0.25	0
7	PG4	F	603	-	12,12,12	0.52	0	11,11,11	0.33	0
6	EDO	F	602	-	3,3,3	0.49	0	2,2,2	0.26	0
5	ETA	B	601	-	3,3,3	0.48	0	2,2,2	0.94	0
10	1PE	E	602	-	15,15,15	0.51	0	14,14,14	0.24	0
3	PGE	A	1802	-	9,9,9	0.33	0	8,8,8	0.29	0
6	EDO	C	1704	-	3,3,3	0.49	0	2,2,2	0.26	0
6	EDO	B	605	-	3,3,3	0.47	0	2,2,2	0.26	0
6	EDO	A	1810	-	3,3,3	0.45	0	2,2,2	0.31	0
6	EDO	A	1808	-	3,3,3	0.41	0	2,2,2	0.39	0
6	EDO	A	1805	-	3,3,3	0.50	0	2,2,2	0.24	0
6	EDO	C	1705	-	3,3,3	0.52	0	2,2,2	0.26	0
7	PG4	A	1811	-	12,12,12	0.53	0	11,11,11	0.41	0
6	EDO	D	603	-	3,3,3	0.51	0	2,2,2	0.10	0
2	P6G	B	606	-	18,18,18	0.53	0	17,17,17	0.25	0
4	PEG	A	1803	-	6,6,6	0.47	0	5,5,5	0.34	0
5	ETA	D	601	-	3,3,3	0.44	0	2,2,2	0.56	0
10	1PE	C	1708	-	15,15,15	0.53	0	14,14,14	0.28	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
6	EDO	C	1706	-	-	0/1/1/1	-
6	EDO	B	603	-	-	0/1/1/1	-
2	P6G	A	1801	-	-	13/16/16/16	-
6	EDO	E	605	-	-	1/1/1/1	-
6	EDO	A	1807	-	-	1/1/1/1	-
6	EDO	C	1707	-	-	1/1/1/1	-
6	EDO	A	1809	-	-	0/1/1/1	-
6	EDO	A	1806	-	-	1/1/1/1	-
7	PG4	F	604	-	-	5/10/10/10	-
5	ETA	F	601	-	-	1/1/1/1	-
5	ETA	A	1804	-	-	1/1/1/1	-
6	EDO	E	603	-	-	1/1/1/1	-
7	PG4	D	604	-	-	5/10/10/10	-
7	PG4	F	605	-	-	5/10/10/10	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	PG4	E	607	-	-	8/10/10/10	-
6	EDO	E	604	-	-	0/1/1/1	-
10	1PE	D	602	-	-	6/13/13/13	-
2	P6G	C	1703	-	-	7/16/16/16	-
7	PG4	B	608	-	-	4/10/10/10	-
6	EDO	B	604	-	-	0/1/1/1	-
5	ETA	C	1702	-	-	1/1/1/1	-
6	EDO	E	606	-	-	0/1/1/1	-
6	EDO	B	602	-	-	0/1/1/1	-
5	ETA	E	601	-	-	1/1/1/1	-
3	PGE	B	607	-	-	4/7/7/7	-
6	EDO	C	1701	-	-	1/1/1/1	-
7	PG4	F	603	-	-	5/10/10/10	-
6	EDO	F	602	-	-	0/1/1/1	-
5	ETA	B	601	-	-	1/1/1/1	-
10	1PE	E	602	-	-	10/13/13/13	-
3	PGE	A	1802	-	-	4/7/7/7	-
6	EDO	C	1704	-	-	1/1/1/1	-
6	EDO	B	605	-	-	0/1/1/1	-
6	EDO	A	1810	-	-	1/1/1/1	-
6	EDO	A	1808	-	-	0/1/1/1	-
6	EDO	A	1805	-	-	0/1/1/1	-
6	EDO	C	1705	-	-	0/1/1/1	-
7	PG4	A	1811	-	-	7/10/10/10	-
6	EDO	D	603	-	-	0/1/1/1	-
2	P6G	B	606	-	-	3/16/16/16	-
4	PEG	A	1803	-	-	1/4/4/4	-
5	ETA	D	601	-	-	1/1/1/1	-
10	1PE	C	1708	-	-	7/13/13/13	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (108) torsion outliers are listed below:

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

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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
2	C	1703	P6G	O13-C14-C15-O16
7	E	607	PG4	O3-C5-C6-O4
3	B	607	PGE	O2-C3-C4-O3
10	D	602	1PE	OH5-C14-C24-OH4
10	C	1708	1PE	OH6-C15-C25-OH5
7	F	604	PG4	O2-C3-C4-O3
2	A	1801	P6G	O13-C14-C15-O16
7	A	1811	PG4	C8-C7-O4-C6
7	F	604	PG4	O3-C5-C6-O4
7	F	603	PG4	O2-C3-C4-O3
7	F	603	PG4	O3-C5-C6-O4
2	C	1703	P6G	O7-C8-C9-O10
2	A	1801	P6G	O4-C5-C6-O7
3	B	607	PGE	O1-C1-C2-O2
7	F	605	PG4	O3-C5-C6-O4
10	E	602	1PE	OH5-C14-C24-OH4
7	E	607	PG4	C5-C6-O4-C7
10	C	1708	1PE	OH5-C14-C24-OH4
4	A	1803	PEG	O2-C3-C4-O4
7	E	607	PG4	O2-C3-C4-O3
10	E	602	1PE	OH6-C15-C25-OH5
2	A	1801	P6G	O1-C2-C3-O4
7	D	604	PG4	O4-C7-C8-O5
7	A	1811	PG4	O3-C5-C6-O4
5	F	601	ETA	O-C-CA-N
10	E	602	1PE	C15-C25-OH5-C14
7	F	603	PG4	C6-C5-O3-C4
7	F	605	PG4	O1-C1-C2-O2
6	C	1701	EDO	O1-C1-C2-O2
7	A	1811	PG4	C6-C5-O3-C4
10	E	602	1PE	C16-C26-OH6-C15
10	E	602	1PE	OH2-C12-C22-OH3
2	B	606	P6G	O16-C17-C18-O19
3	A	1802	PGE	O3-C5-C6-O4
6	C	1707	EDO	O1-C1-C2-O2
2	A	1801	P6G	C5-C6-O7-C8
3	A	1802	PGE	O2-C3-C4-O3
5	A	1804	ETA	O-C-CA-N
2	C	1703	P6G	O4-C5-C6-O7

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Mol	Chain	Res	Type	Atoms
2	A	1801	P6G	C12-C11-O10-C9
2	A	1801	P6G	O7-C8-C9-O10
10	D	602	1PE	OH6-C15-C25-OH5
6	A	1810	EDO	O1-C1-C2-O2
7	A	1811	PG4	O2-C3-C4-O3
7	A	1811	PG4	C3-C4-O3-C5
7	E	607	PG4	C6-C5-O3-C4
7	F	605	PG4	C5-C6-O4-C7
2	A	1801	P6G	C9-C8-O7-C6
7	F	604	PG4	C3-C4-O3-C5
7	D	604	PG4	C3-C4-O3-C5
10	C	1708	1PE	C24-C14-OH5-C25
2	B	606	P6G	C15-C14-O13-C12
7	F	604	PG4	C8-C7-O4-C6
2	A	1801	P6G	C18-C17-O16-C15
7	E	607	PG4	C1-C2-O2-C3
7	E	607	PG4	C4-C3-O2-C2
2	B	606	P6G	C2-C3-O4-C5
10	D	602	1PE	C16-C26-OH6-C15
10	C	1708	1PE	C12-C22-OH3-C23
3	A	1802	PGE	O1-C1-C2-O2
7	D	604	PG4	O1-C1-C2-O2
2	A	1801	P6G	C6-C5-O4-C3
10	E	602	1PE	C24-C14-OH5-C25
10	C	1708	1PE	C23-C13-OH4-C24
10	D	602	1PE	C25-C15-OH6-C26
10	E	602	1PE	OH4-C13-C23-OH3
7	B	608	PG4	O4-C7-C8-O5
7	F	603	PG4	O1-C1-C2-O2
6	A	1806	EDO	O1-C1-C2-O2
6	A	1807	EDO	O1-C1-C2-O2
6	E	605	EDO	O1-C1-C2-O2
2	A	1801	P6G	C14-C15-O16-C17
2	A	1801	P6G	C8-C9-O10-C11
5	E	601	ETA	O-C-CA-N
2	A	1801	P6G	O10-C11-C12-O13
7	E	607	PG4	C3-C4-O3-C5
3	B	607	PGE	C1-C2-O2-C3
7	B	608	PG4	C1-C2-O2-C3
7	B	608	PG4	O1-C1-C2-O2
10	E	602	1PE	C14-C24-OH4-C13
7	E	607	PG4	O4-C7-C8-O5

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Mol	Chain	Res	Type	Atoms
6	E	603	EDO	O1-C1-C2-O2
7	F	605	PG4	C8-C7-O4-C6
7	F	603	PG4	C1-C2-O2-C3
5	C	1702	ETA	O-C-CA-N
2	C	1703	P6G	C5-C6-O7-C8
7	A	1811	PG4	O1-C1-C2-O2
10	E	602	1PE	C23-C13-OH4-C24
7	F	604	PG4	C1-C2-O2-C3
7	B	608	PG4	C4-C3-O2-C2
2	C	1703	P6G	C6-C5-O4-C3
10	C	1708	1PE	C16-C26-OH6-C15
10	D	602	1PE	C23-C13-OH4-C24
6	C	1704	EDO	O1-C1-C2-O2
2	A	1801	P6G	O16-C17-C18-O19
3	B	607	PGE	O3-C5-C6-O4
3	A	1802	PGE	C4-C3-O2-C2
7	F	605	PG4	O2-C3-C4-O3
7	D	604	PG4	O3-C5-C6-O4
2	C	1703	P6G	C8-C9-O10-C11
10	C	1708	1PE	OH4-C13-C23-OH3
7	D	604	PG4	O2-C3-C4-O3
10	D	602	1PE	OH4-C13-C23-OH3

There are no ring outliers.

25 monomers are involved in 47 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	1706	EDO	1	0
2	A	1801	P6G	1	0
6	A	1809	EDO	1	0
7	F	604	PG4	1	0
5	A	1804	ETA	1	0
6	E	603	EDO	2	0
7	D	604	PG4	4	0
7	F	605	PG4	1	0
7	E	607	PG4	3	0
6	E	604	EDO	2	0
10	D	602	1PE	2	0
2	C	1703	P6G	1	0
7	B	608	PG4	3	0
6	B	604	EDO	2	0
6	C	1701	EDO	1	0

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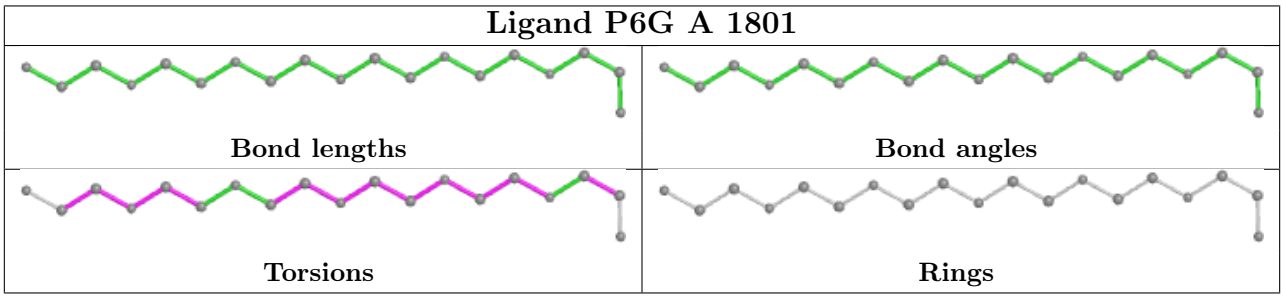
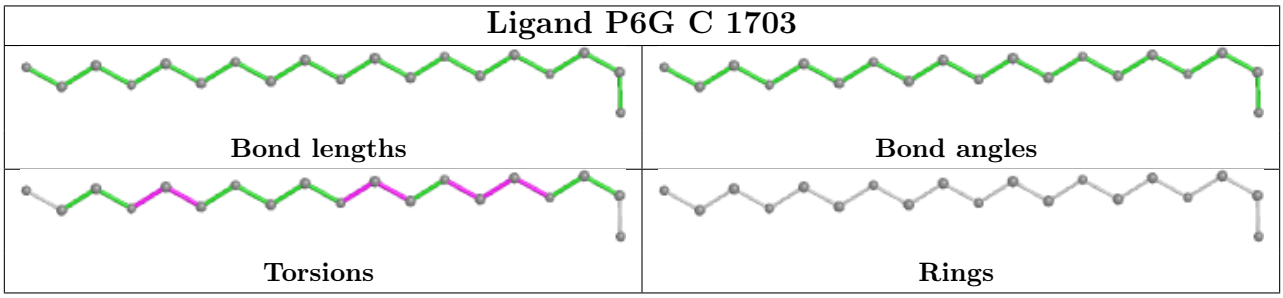
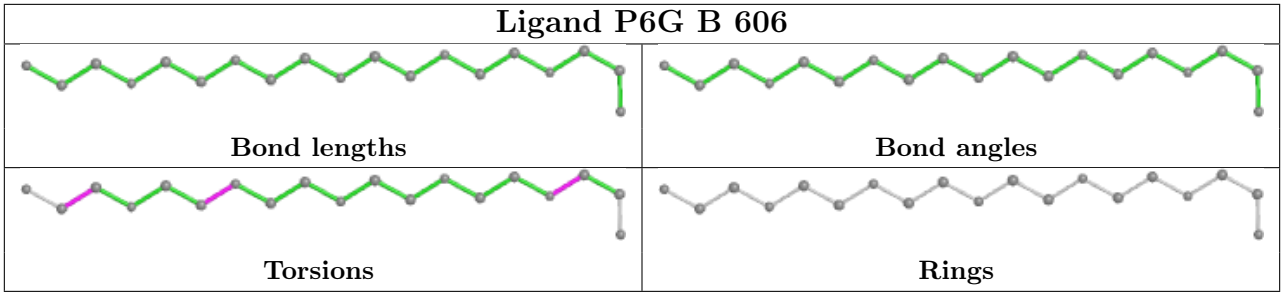
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	F	603	PG4	5	0
6	C	1704	EDO	1	0
6	B	605	EDO	1	0
6	A	1810	EDO	2	0
6	A	1808	EDO	1	0
6	C	1705	EDO	2	0
7	A	1811	PG4	2	0
6	D	603	EDO	1	0
2	B	606	P6G	3	0
10	C	1708	1PE	4	0

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 then 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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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%)	-0.04	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

All (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
1	D	369	THR	9.6
1	B	586	ASN	9.4
1	E	387	ALA	9.1
1	A	586	ASN	8.7
1	F	586	ASN	8.7
1	D	586	ASN	8.2
1	A	243	SER	7.9
1	C	367	ALA	7.4
1	D	387	ALA	7.0
1	C	410	LYS	6.7
1	B	384	GLY	6.7
1	E	586	ASN	6.6
1	A	407	SER	6.3
1	E	367	ALA	6.2

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Mol	Chain	Res	Type	RSRZ
1	E	368	GLN	6.2
1	C	349	ALA	6.1
1	B	369	THR	5.9
1	A	585	ALA	5.9
1	A	409	GLN	5.8
1	D	367	ALA	5.7
1	B	368	GLN	5.7
1	A	367	ALA	5.6
1	C	406	ASP	5.6
1	F	369	THR	5.5
1	F	405	ASP	5.2
1	F	408	ASN	5.2
1	C	585	ALA	5.0
1	C	243	SER	4.9
1	A	386	TYR	4.7
1	A	406	ASP	4.6
1	C	369	THR	4.5
1	E	406	ASP	4.5
1	F	366	ALA	4.4
1	E	389	GLU	4.3
1	F	411	ASN	4.3
1	C	408	ASN	4.3
1	B	390	ASP	4.3
1	B	367	ALA	4.1
1	D	366	ALA	4.1
1	C	409	GLN	4.1
1	E	390	ASP	4.1
1	B	366	ALA	4.0
1	D	564	LYS	4.0
1	D	405	ASP	3.9
1	A	410	LYS	3.9
1	E	369	THR	3.8
1	B	385	ARG	3.8
1	F	388	GLN	3.7
1	E	349	ALA	3.7
1	F	347	ASP	3.7
1	A	390	ASP	3.7
1	D	347	ASP	3.6
1	F	389	GLU	3.5
1	B	388	GLN	3.5
1	B	564	LYS	3.5
1	C	347	ASP	3.4

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Mol	Chain	Res	Type	RSRZ
1	E	405	ASP	3.4
1	F	367	ALA	3.4
1	F	409	GLN	3.3
1	E	412	PHE	3.2
1	A	388	GLN	3.2
1	D	389	GLU	3.2
1	F	368	GLN	3.2
1	E	410	LYS	3.1
1	F	564	LYS	3.1
1	A	349	ALA	3.0
1	D	349	ALA	3.0
1	D	406	ASP	3.0
1	E	348	GLY	2.9
1	C	348	GLY	2.9
1	D	414	LYS	2.9
1	D	565	ASP	2.9
1	F	406	ASP	2.9
1	E	564	LYS	2.9
1	C	368	GLN	2.8
1	C	407	SER	2.8
1	C	366	ALA	2.7
1	F	412	PHE	2.7
1	A	387	ALA	2.7
1	A	414	LYS	2.7
1	A	348	GLY	2.7
1	F	390	ASP	2.6
1	A	389	GLU	2.6
1	B	389	GLU	2.6
1	E	385	ARG	2.6
1	B	386	TYR	2.6
1	B	349	ALA	2.6
1	A	346	SER	2.5
1	A	368	GLN	2.5
1	A	369	THR	2.5
1	F	404	ILE	2.5
1	E	347	ASP	2.5
1	E	388	GLN	2.5
1	E	414	LYS	2.4
1	A	244	VAL	2.4
1	D	385	ARG	2.4
1	A	347	ASP	2.4
1	E	408	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
1	E	366	ALA	2.3
1	F	414	LYS	2.3
1	D	390	ASP	2.2
1	B	526	ASN	2.2
1	D	365	PRO	2.2
1	B	585	ALA	2.2
1	D	243	SER	2.2
1	A	408	ASN	2.1
1	F	348	GLY	2.1
1	C	350	ALA	2.1
1	D	256	MET	2.1
1	B	409	GLN	2.1
1	E	552	HIS	2.0
1	F	565	ASP	2.0
1	B	405	ASP	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no 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, 95^{th} 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
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
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	C	1704	4/4	0.79	0.17	57,61,65,67	0
6	EDO	A	1806	4/4	0.79	0.18	46,52,53,55	0
3	PGE	B	607	10/10	0.80	0.15	72,73,74,74	0
3	PGE	A	1802	10/10	0.80	0.15	56,60,67,68	0
7	PG4	F	605	13/13	0.81	0.16	59,70,74,75	0
7	PG4	F	603	13/13	0.81	0.14	61,66,76,76	0
2	P6G	B	606	19/19	0.82	0.17	41,53,71,71	0
2	P6G	C	1703	19/19	0.83	0.14	50,63,68,69	0
6	EDO	B	602	4/4	0.83	0.44	71,72,72,72	0
2	P6G	A	1801	19/19	0.83	0.14	54,62,75,75	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	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	B	604	4/4	0.86	0.30	44,51,52,54	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
5	ETA	E	601	4/4	0.89	0.14	36,39,41,47	0
7	PG4	B	608	13/13	0.89	0.12	46,48,63,63	0
6	EDO	B	603	4/4	0.89	0.28	44,53,62,70	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
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
9	K	D	606	1/1	0.97	0.08	61,61,61,61	0
8	MG	C	1709	1/1	0.97	0.14	33,33,33,33	0
5	ETA	C	1702	4/4	0.97	0.08	29,32,32,33	0
8	MG	F	606	1/1	0.97	0.11	45,45,45,45	0
8	MG	E	608	1/1	0.98	0.05	43,43,43,43	0
9	K	B	610	1/1	0.98	0.08	56,56,56,56	0
9	K	A	1813	1/1	0.99	0.27	43,43,43,43	0

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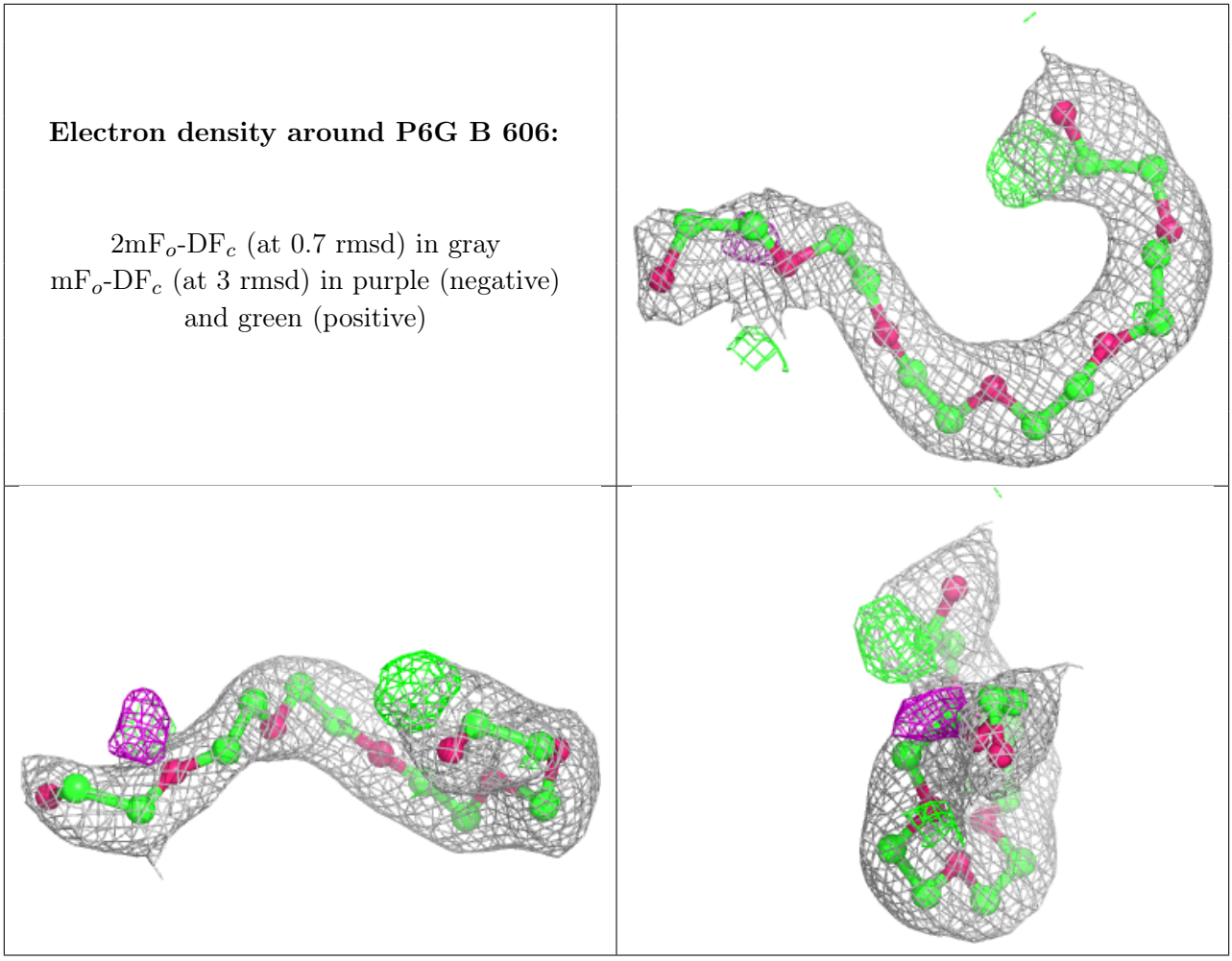
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
8	MG	A	1812	1/1	0.99	0.10	31,31,31,31	0
8	MG	B	609	1/1	0.99	0.14	33,33,33,33	0

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.

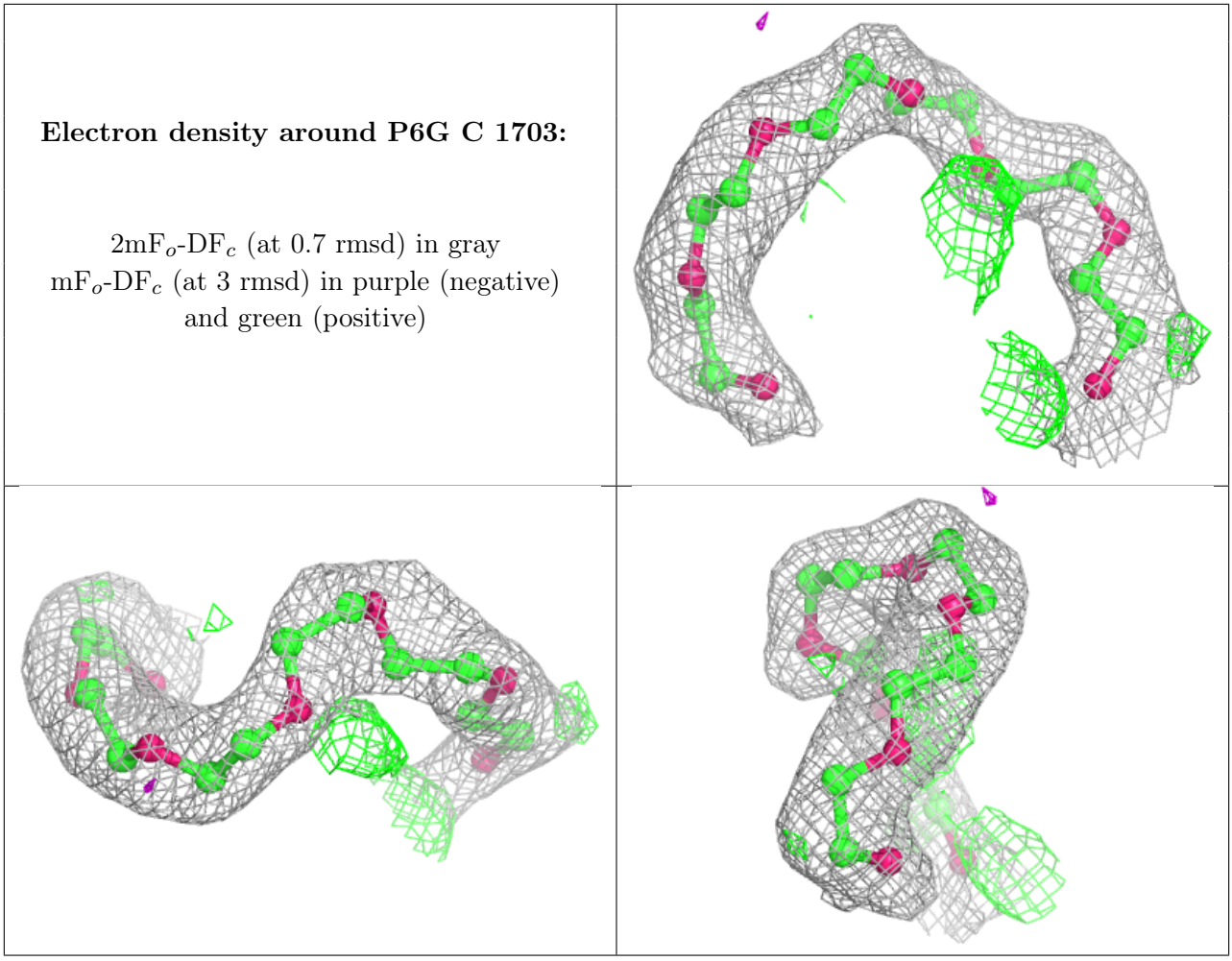
Electron density around P6G B 606:

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



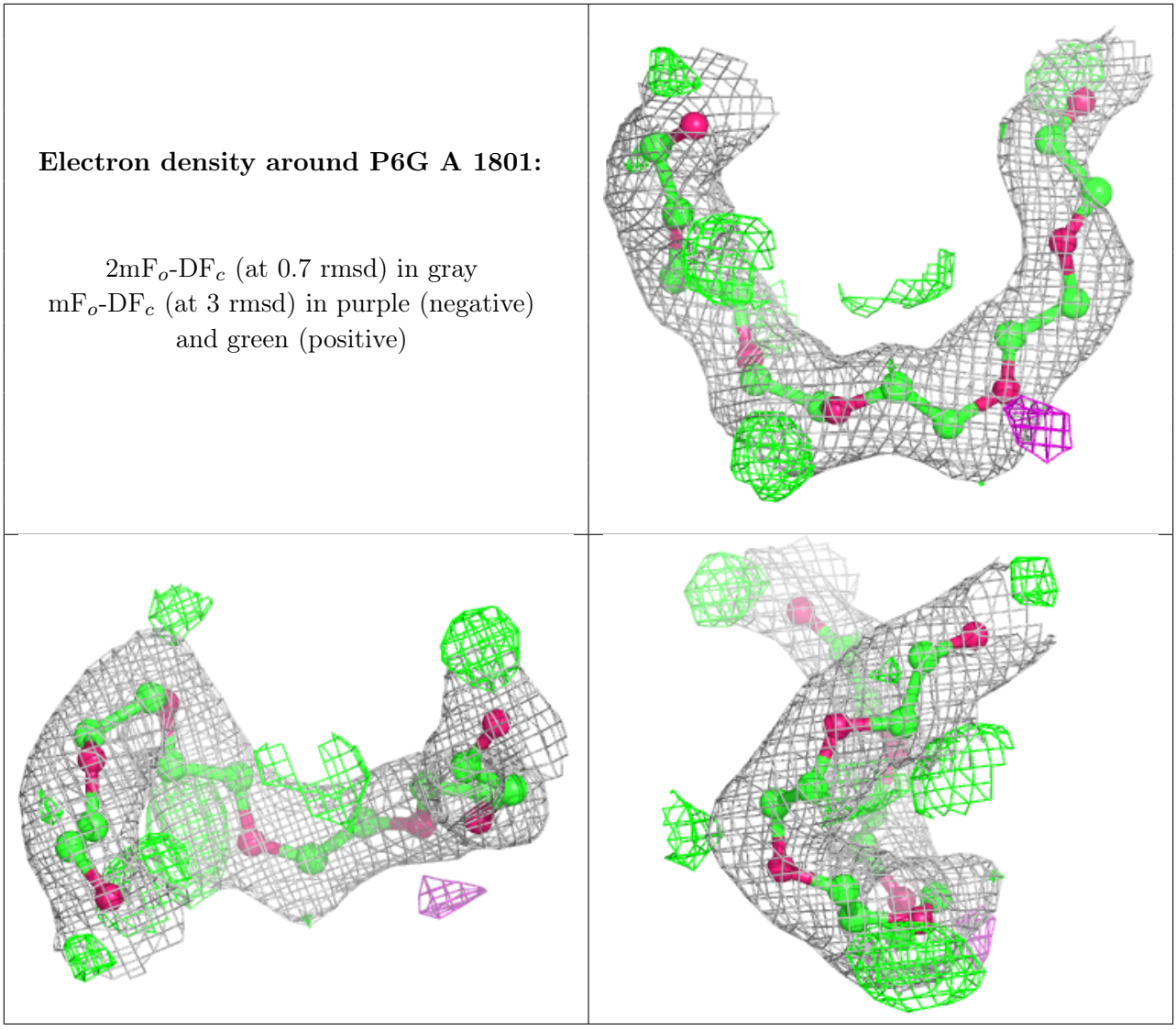
Electron density around P6G C 1703:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (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.