



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 26, 2020 – 09:00 am BST

PDB ID : 6CJ6  
Title : Structure of the poxvirus protein F9  
Authors : Diesterbeck, U.S.; Gittis, A.G.; Garboczi, D.N.; Moss, B.  
Deposited on : 2018-02-26  
Resolution : 2.10 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 : 2.11  
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) : 2.11

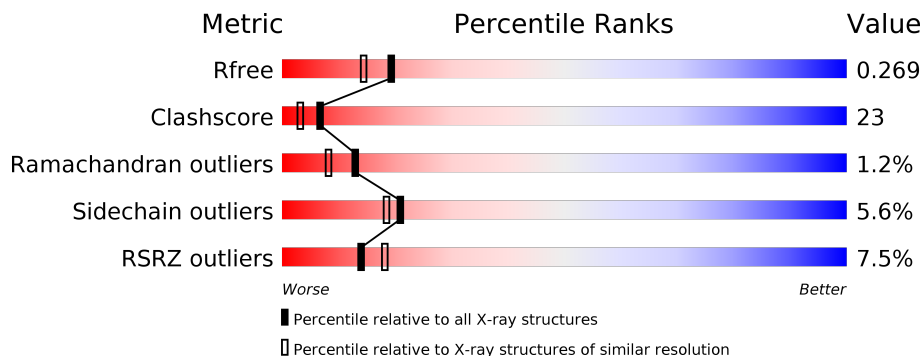
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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	176	 10% 64% 28% • 6%
1	B	176	 6% 65% 22% 5% 9%
1	C	176	 6% 68% 22% • 9%
1	D	176	 7% 66% 26% • 6%

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

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	PGO	A	247	-	-	X	-
10	PGO	B	230	X	-	-	-
10	PGO	D	245	-	-	X	-
10	PGO	D	246	-	-	X	-
11	ETX	A	250	-	-	X	-
11	ETX	B	236	-	-	-	X
11	ETX	C	242	-	-	-	X
11	ETX	D	249	-	-	X	-
11	ETX	D	250	-	-	X	-
14	P33	C	207	-	-	X	-
15	P6G	D	209	-	-	X	-
2	PG4	D	202	-	-	X	-
3	PG0	A	204	-	-	X	-
4	PEG	A	207	-	-	X	-
4	PEG	C	203	-	-	X	-
4	PEG	C	205	-	X	X	-
4	PEG	D	205	-	-	X	-
4	PEG	D	206	-	-	X	X
5	EDO	A	213	-	-	-	X
5	EDO	B	209	-	-	-	X
5	EDO	D	216	-	-	-	X
5	EDO	D	220	-	-	-	X
6	GOL	A	218	-	X	-	-
6	GOL	C	216	-	-	-	X
6	GOL	C	217	-	X	-	-
6	GOL	C	218	-	X	-	-
6	GOL	C	219	-	X	-	-
7	PDO	A	221	-	-	X	-
7	PDO	D	224	-	-	X	-
8	EOH	A	226	-	-	X	-
8	EOH	A	236	-	-	X	-
8	EOH	B	217	-	-	X	-
8	EOH	B	220	-	-	X	-
8	EOH	B	223	-	-	X	-
8	EOH	C	225	-	-	X	-
8	EOH	C	226	-	-	X	-
8	EOH	C	230	-	-	-	X
8	EOH	D	230	-	-	X	-
9	MOH	A	243	-	-	-	X
9	MOH	B	229	-	-	X	-

## 2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 6060 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Protein F9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	165	1239	784	206	240	9	0	0	0
1	B	161	1210	764	202	235	9	0	0	0
1	C	161	1225	771	204	241	9	0	1	0
1	D	166	1271	801	214	246	10	0	1	0

There are 8 discrepancies between the modelled and reference sequences:

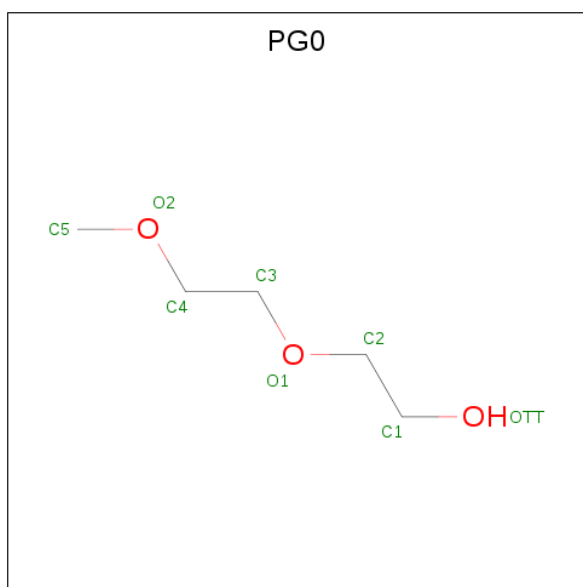
Chain	Residue	Modelled	Actual	Comment	Reference
A	84	ALA	ARG	conflict	UNP P24361
A	147	ALA	ARG	conflict	UNP P24361
B	84	ALA	ARG	conflict	UNP P24361
B	147	ALA	ARG	conflict	UNP P24361
C	84	ALA	ARG	conflict	UNP P24361
C	147	ALA	ARG	conflict	UNP P24361
D	84	ALA	ARG	conflict	UNP P24361
D	147	ALA	ARG	conflict	UNP P24361

- Molecule 2 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
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	D	1	Total	C	O	0	0
			13	8	5		
2	D	1	Total	C	O	0	0
			13	8	5		

- Molecule 3 is 2-(2-METHOXYETHOXY)ETHANOL (three-letter code: PG0) (formula: C<sub>5</sub>H<sub>12</sub>O<sub>3</sub>).



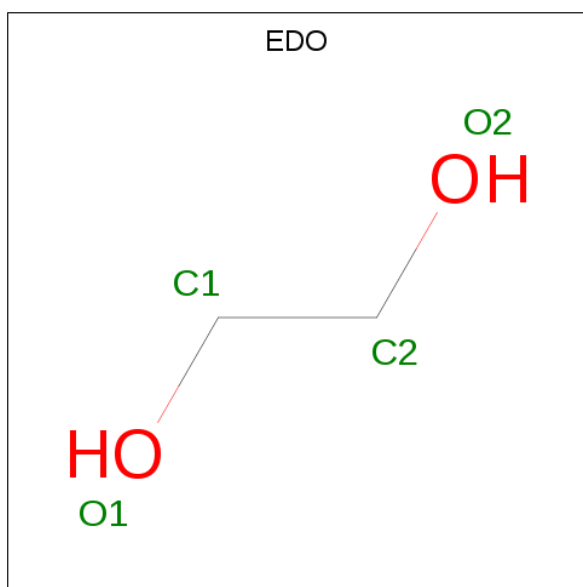
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			8	5	3		
3	A	1	Total	C	O	0	0
			8	5	3		
3	A	1	Total	C	O	0	0
			8	5	3		
3	A	1	Total	C	O	0	0
			8	5	3		
3	B	1	Total	C	O	0	0
			8	5	3		
3	C	1	Total	C	O	0	0
			8	5	3		
3	C	1	Total	C	O	0	0
			8	5	3		
3	D	1	Total	C	O	0	0
			8	5	3		
3	D	1	Total	C	O	0	0
			8	5	3		

- Molecule 4 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>3</sub>).



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

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



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

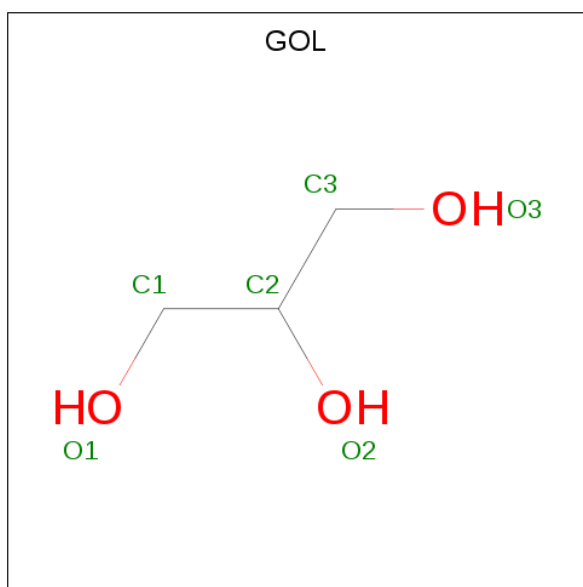
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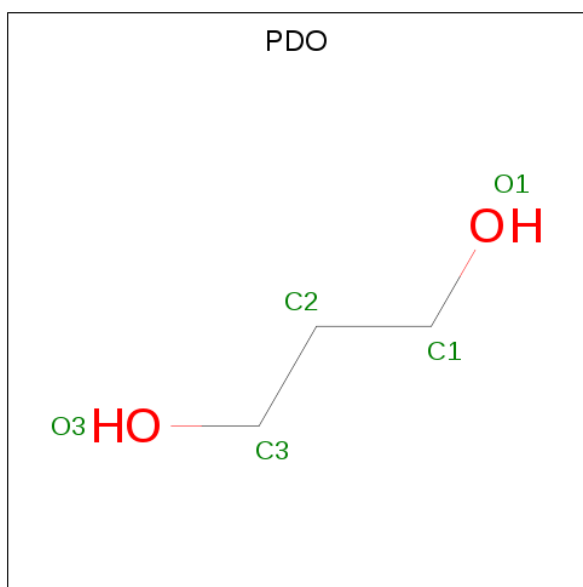
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total C O 4 2 2	0	0
5	C	1	Total C O 4 2 2	0	0
5	C	1	Total C O 4 2 2	0	0
5	C	1	Total C O 4 2 2	0	0
5	C	1	Total C O 4 2 2	0	0
5	C	1	Total C O 4 2 2	0	0
5	C	1	Total C O 4 2 2	0	0
5	C	1	Total C O 4 2 2	0	0
5	D	1	Total C O 4 2 2	0	0
5	D	1	Total C O 4 2 2	0	0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

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



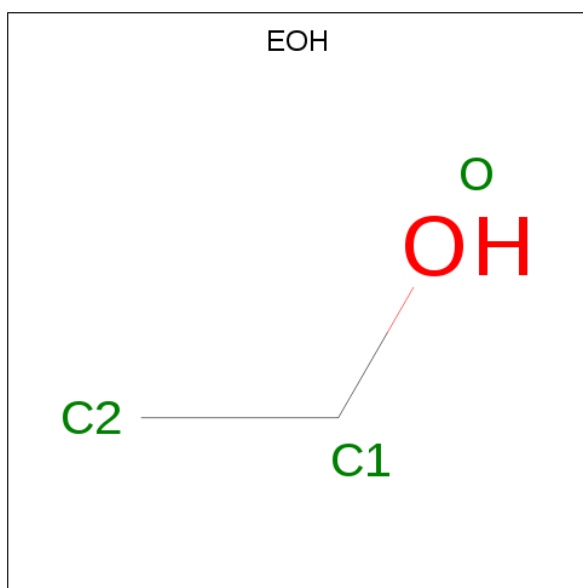
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			6	3	3		
6	C	1	Total	C	O	0	0
			6	3	3		
6	C	1	Total	C	O	0	0
			6	3	3		
6	C	1	Total	C	O	0	0
			6	3	3		
6	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 7 is 1,3-PROPANDIOL (three-letter code: PDO) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C O 5 3 2	0	0
7	A	1	Total C O 5 3 2	0	0
7	A	1	Total C O 5 3 2	0	0
7	A	1	Total C O 5 3 2	0	0
7	A	1	Total C O 5 3 2	0	0
7	A	1	Total C O 5 3 2	0	0
7	A	1	Total C O 5 3 2	0	0
7	B	1	Total C O 5 3 2	0	0
7	B	1	Total C O 5 3 2	0	0
7	B	1	Total C O 5 3 2	0	0
7	C	1	Total C O 5 3 2	0	0
7	C	1	Total C O 5 3 2	0	0
7	D	1	Total C O 5 3 2	0	0
7	D	1	Total C O 5 3 2	0	0

- Molecule 8 is ETHANOL (three-letter code: EOH) (formula: C<sub>2</sub>H<sub>6</sub>O).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C O 3 2 1	0	0
8	A	1	Total C O 3 2 1	0	0
8	A	1	Total C O 3 2 1	0	0
8	A	1	Total C O 3 2 1	0	0
8	A	1	Total C O 3 2 1	0	0
8	A	1	Total C O 3 2 1	0	0
8	A	1	Total C O 3 2 1	0	0
8	A	1	Total C O 3 2 1	0	0
8	A	1	Total C O 3 2 1	0	0
8	A	1	Total C O 3 2 1	0	0
8	A	1	Total C O 3 2 1	0	0
8	A	1	Total C O 3 2 1	0	0
8	A	1	Total C O 3 2 1	0	0
8	A	1	Total C O 3 2 1	0	0

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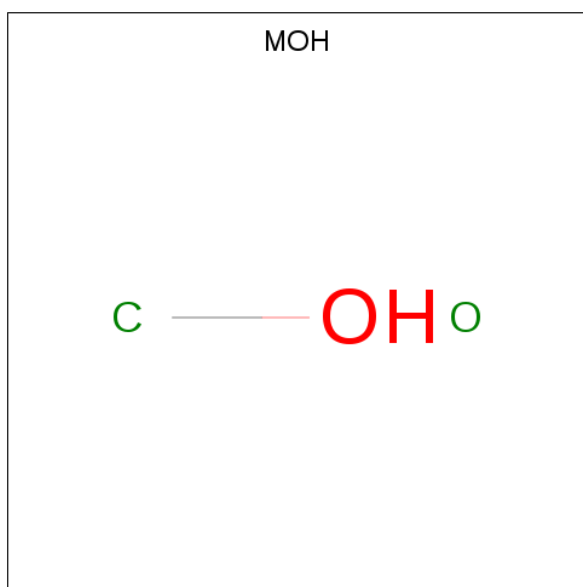
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	C	O	0	0
			3	2	1		
8	B	1	Total	C	O	0	0
			3	2	1		
8	B	1	Total	C	O	0	0
			3	2	1		
8	B	1	Total	C	O	0	0
			3	2	1		
8	B	1	Total	C	O	0	0
			3	2	1		
8	B	1	Total	C	O	0	0
			3	2	1		
8	B	1	Total	C	O	0	0
			3	2	1		
8	B	1	Total	C	O	0	0
			3	2	1		
8	B	1	Total	C	O	0	0
			3	2	1		
8	B	1	Total	C	O	0	0
			3	2	1		
8	C	1	Total	C	O	0	0
			3	2	1		
8	C	1	Total	C	O	0	0
			3	2	1		
8	C	1	Total	C	O	0	0
			3	2	1		
8	C	1	Total	C	O	0	0
			3	2	1		
8	C	1	Total	C	O	0	0
			3	2	1		
8	C	1	Total	C	O	0	0
			3	2	1		
8	C	1	Total	C	O	0	0
			3	2	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	C	1	Total 3	C 2	O 1	0	0
8	D	1	Total 3	C 2	O 1	0	0
8	D	1	Total 3	C 2	O 1	0	0
8	D	1	Total 3	C 2	O 1	0	0
8	D	1	Total 3	C 2	O 1	0	0
8	D	1	Total 3	C 2	O 1	0	0
8	D	1	Total 3	C 2	O 1	0	0
8	D	1	Total 3	C 2	O 1	0	0
8	D	1	Total 3	C 2	O 1	0	0
8	D	1	Total 3	C 2	O 1	0	0
8	D	1	Total 3	C 2	O 1	0	0
8	D	1	Total 3	C 2	O 1	0	0
8	D	1	Total 3	C 2	O 1	0	0
8	D	1	Total 3	C 2	O 1	0	0

- Molecule 9 is METHANOL (three-letter code: MOH) (formula: CH<sub>4</sub>O).



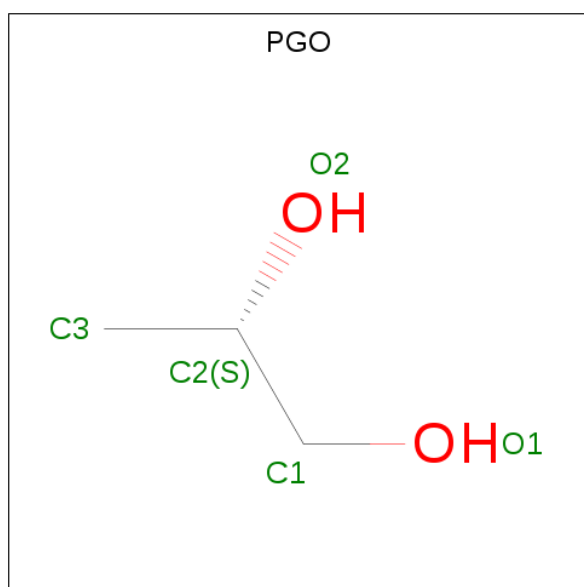
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	C	O	0	0
			2	1	1		
9	A	1	Total	C	O	0	0
			2	1	1		
9	A	1	Total	C	O	0	0
			2	1	1		
9	A	1	Total	C	O	0	0
			2	1	1		
9	A	1	Total	C	O	0	0
			2	1	1		
9	A	1	Total	C	O	0	0
			2	1	1		
9	A	1	Total	C	O	0	0
			2	1	1		
9	B	1	Total	C	O	0	0
			2	1	1		
9	B	1	Total	C	O	0	0
			2	1	1		
9	B	1	Total	C	O	0	0
			2	1	1		
9	C	1	Total	C	O	0	0
			2	1	1		
9	C	1	Total	C	O	0	0
			2	1	1		
9	C	1	Total	C	O	0	0
			2	1	1		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	C	1	Total C O 2 1 1	0	0
9	C	1	Total C O 2 1 1	0	0
9	C	1	Total C O 2 1 1	0	0
9	D	1	Total C O 2 1 1	0	0
9	D	1	Total C O 2 1 1	0	0
9	D	1	Total C O 2 1 1	0	0
9	D	1	Total C O 2 1 1	0	0
9	D	1	Total C O 2 1 1	0	0
9	D	1	Total C O 2 1 1	0	0
9	D	1	Total C O 2 1 1	0	0
9	D	1	Total C O 2 1 1	0	0

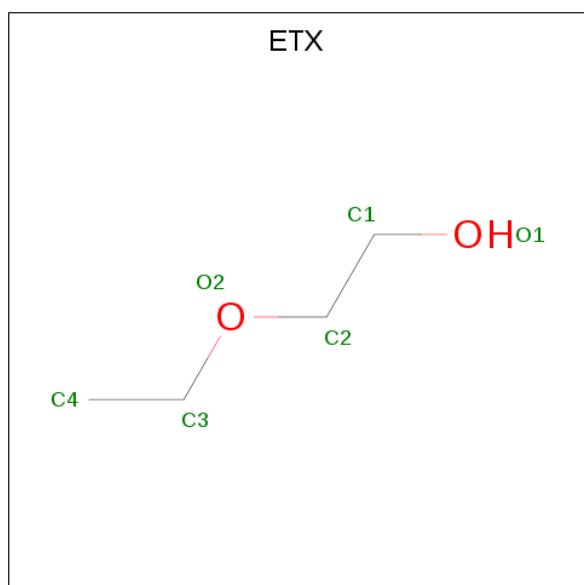
- Molecule 10 is S-1,2-PROPANEDIOL (three-letter code: PGO) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>2</sub>).





Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	A	1	Total	C	O	0	0
			5	3	2		
10	A	1	Total	C	O	0	0
			5	3	2		
10	A	1	Total	C	O	0	0
			5	3	2		
10	B	1	Total	C	O	0	0
			5	3	2		
10	B	1	Total	C	O	0	0
			5	3	2		
10	B	1	Total	C	O	0	0
			5	3	2		
10	C	1	Total	C	O	0	0
			5	3	2		
10	D	1	Total	C	O	0	0
			5	3	2		
10	D	1	Total	C	O	0	0
			5	3	2		
10	D	1	Total	C	O	0	0
			5	3	2		

- Molecule 11 is 2-ETHOXYETHANOL (three-letter code: ETX) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>2</sub>).



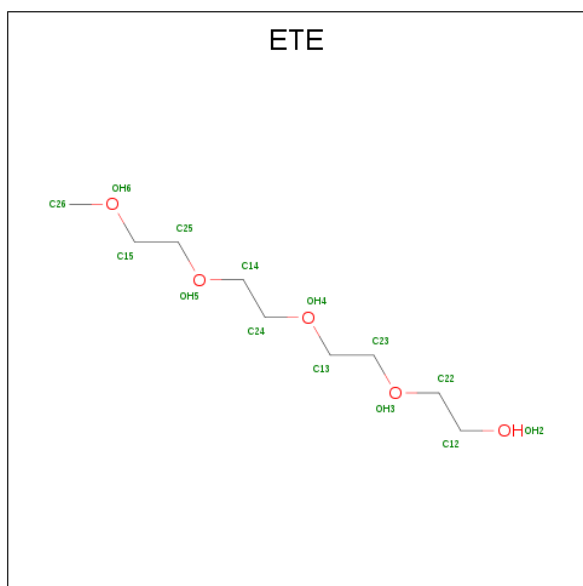
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	A	1	Total	C	O	0	0
			6	4	2		
11	A	1	Total	C	O	0	0
			6	4	2		

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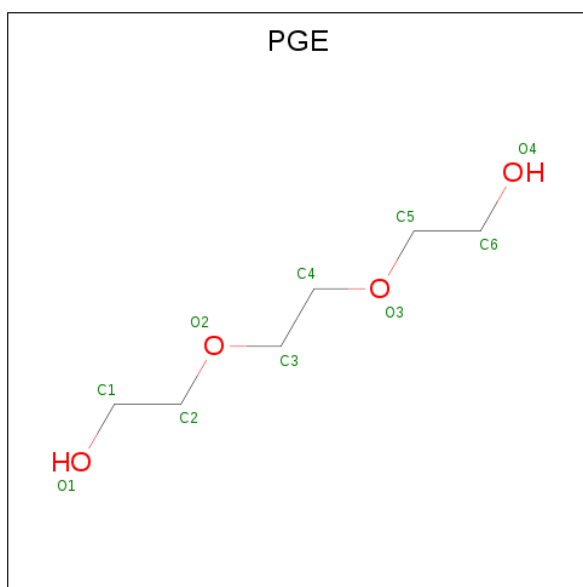
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	B	1	Total	C	O	0	0
			6	4	2		
11	B	1	Total	C	O	0	0
			6	4	2		
11	B	1	Total	C	O	0	0
			6	4	2		
11	C	1	Total	C	O	0	0
			6	4	2		
11	D	1	Total	C	O	0	0
			6	4	2		
11	D	1	Total	C	O	0	0
			6	4	2		

- Molecule 12 is 2-{2-[2-2-(METHOXY-ETHOXY)-ETHOXY]-ETHOXY}-ETHANOL (three-letter code: ETE) (formula: C<sub>9</sub>H<sub>20</sub>O<sub>5</sub>).



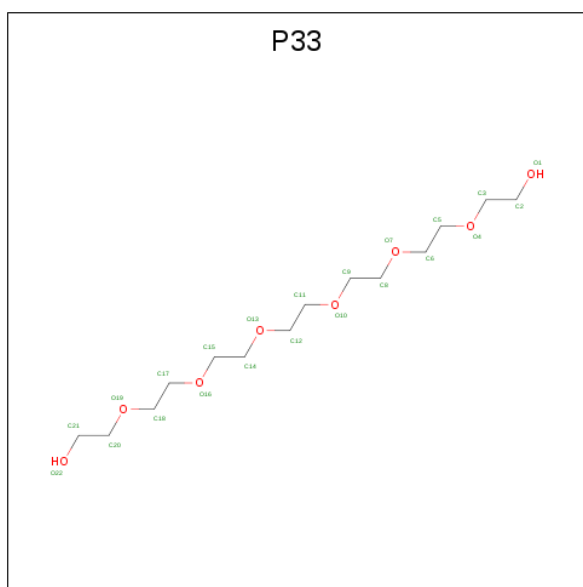
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	B	1	Total	C	O	0	0
			14	9	5		
12	C	1	Total	C	O	0	0
			14	9	5		

- Molecule 13 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: C<sub>6</sub>H<sub>14</sub>O<sub>4</sub>).



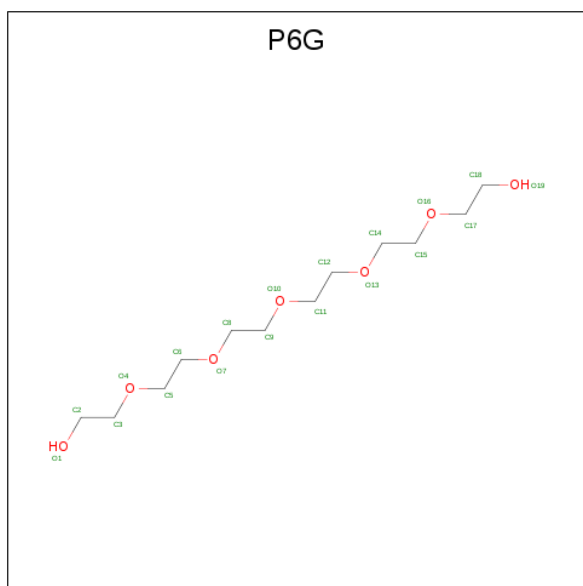
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	B	1	Total C O 10 6 4	0	0
13	C	1	Total C O 10 6 4	0	0
13	C	1	Total C O 10 6 4	0	0
13	C	1	Total C O 10 6 4	0	0
13	D	1	Total C O 10 6 4	0	0

- Molecule 14 is 3,6,9,12,15,18-HEXAOXAIICOSANE-1,20-DIOL (three-letter code: P33) (formula: C<sub>14</sub>H<sub>30</sub>O<sub>8</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
14	C	1	Total	C	O	0	0
			22	14	8		

- Molecule 15 is HEXAETHYLENE GLYCOL (three-letter code: P6G) (formula: C<sub>12</sub>H<sub>26</sub>O<sub>7</sub>).



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

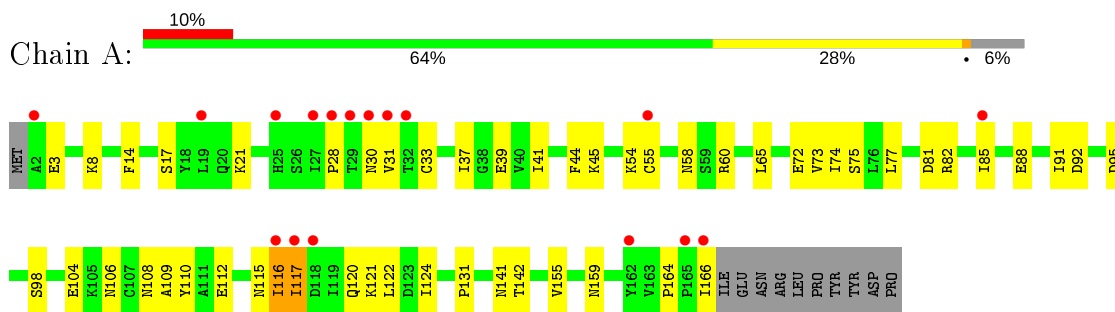
- Molecule 16 is water.

<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
16	A	53	Total 53	O 53	0	0
16	B	60	Total 60	O 60	0	0
16	C	57	Total 58	O 58	0	1
16	D	46	Total 46	O 46	0	0

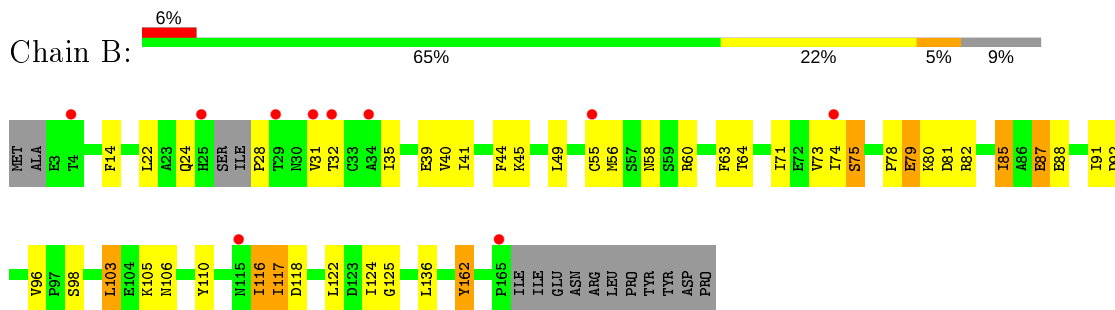
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

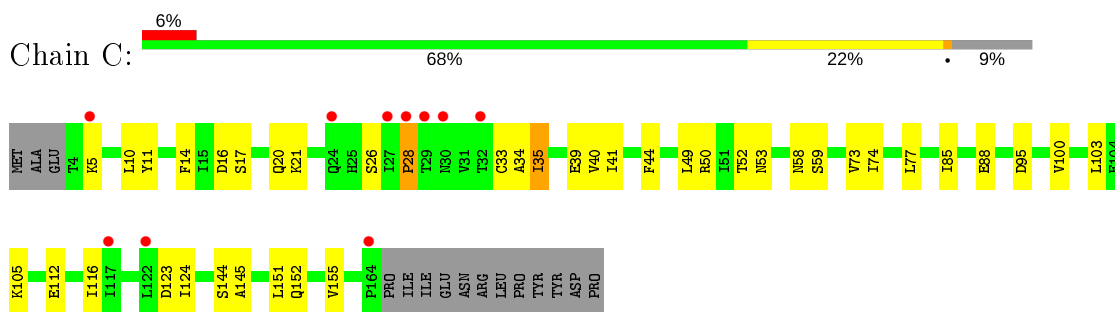
- Molecule 1: Protein F9



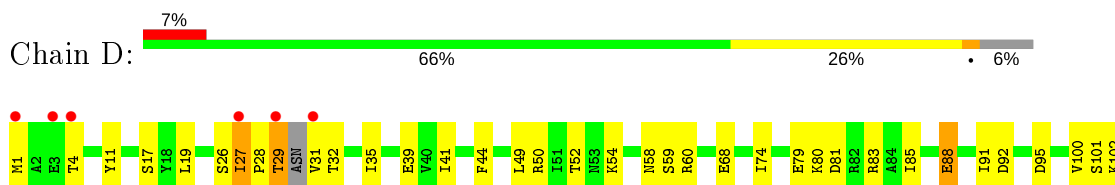
- Molecule 1: Protein F9

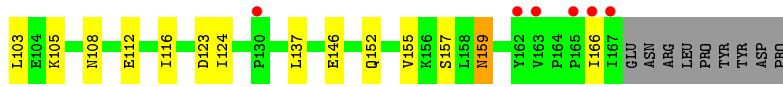


- Molecule 1: Protein F9



- Molecule 1: Protein F9





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	65.45Å 75.08Å 136.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.86 – 2.10 39.96 – 2.10	Depositor EDS
% Data completeness (in resolution range)	93.8 (38.86-2.10) 93.9 (39.96-2.10)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.20 (at 2.10Å)	Xtrriage
Refinement program	PHENIX (1.12_2829)	Depositor
R, $R_{free}$	0.226 , 0.269 0.226 , 0.269	Depositor DCC
$R_{free}$ test set	2000 reflections (5.33%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	30.5	Xtrriage
Anisotropy	0.854	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 68.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	6060	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	42.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 31.08 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.1740e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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: GOL, PGE, P6G, PGO, ETX, EOH, EDO, PDO, PG4, MOH, PG0, ETE, P33, 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	0.32	0/1257	0.44	0/1706
1	B	0.39	1/1225 (0.1%)	0.51	1/1659 (0.1%)
1	C	0.35	0/1240	0.49	1/1680 (0.1%)
1	D	0.28	0/1287	0.48	0/1742
All	All	0.34	1/5009 (0.0%)	0.48	2/6787 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	162	TYR	CB-CG	-6.29	1.42	1.51

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	28	PRO	N-CA-CB	6.10	110.62	103.30
1	B	28	PRO	N-CA-CB	5.91	110.39	103.30

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	1239	0	1217	49	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1210	0	1189	34	0
1	C	1225	0	1198	41	0
1	D	1271	0	1264	65	0
2	A	26	0	36	1	0
2	B	13	0	17	2	0
2	D	26	0	35	9	0
3	A	32	0	48	16	0
3	B	8	0	12	2	0
3	C	16	0	24	8	0
3	D	16	0	24	9	0
4	A	14	0	20	4	0
4	B	14	0	20	0	0
4	C	28	0	39	13	0
4	D	21	0	30	12	0
5	A	36	0	53	7	0
5	B	24	0	35	5	0
5	C	28	0	36	6	0
5	D	44	0	64	3	0
6	A	6	0	6	0	0
6	C	24	0	29	2	0
6	D	6	0	6	2	0
7	A	35	0	54	13	0
7	B	15	0	24	1	0
7	C	10	0	16	1	0
7	D	10	0	16	11	0
8	A	39	0	76	6	0
8	B	36	0	70	7	0
8	C	30	0	60	11	0
8	D	36	0	70	12	0
9	A	16	0	0	0	0
9	B	6	0	0	2	0
9	C	12	0	0	0	0
9	D	16	0	0	2	0
10	A	15	0	24	11	0
10	B	15	0	22	2	0
10	C	5	0	7	0	0
10	D	15	0	23	9	0
11	A	12	0	19	8	0
11	B	18	0	30	3	0
11	C	6	0	10	0	0
11	D	12	0	20	16	0
12	B	14	0	20	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	C	14	0	20	1	0
13	B	10	0	14	3	0
13	C	30	0	41	8	0
13	D	10	0	14	1	0
14	C	22	0	30	14	0
15	D	57	0	78	22	0
16	A	53	0	0	3	0
16	B	60	0	0	2	0
16	C	58	0	0	6	0
16	D	46	0	0	1	0
All	All	6060	0	6160	281	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 23.

The worst 5 of 281 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:D:101:SER:HA	7:D:224:PDO:H32	1.21	1.16
4:A:207:PEG:H11	7:A:219:PDO:H31	1.22	1.15
10:A:247:PGO:C3	11:A:250:ETX:H12	1.78	1.12
12:B:205:ETE:H141	11:D:250:ETX:H41	1.20	1.11
10:A:247:PGO:H31	11:A:250:ETX:H12	1.17	1.09

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	163/176 (93%)	151 (93%)	10 (6%)	2 (1%)	<b>13</b> <b>8</b>
1	B	157/176 (89%)	144 (92%)	9 (6%)	4 (2%)	<b>5</b> <b>2</b>

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	160/176 (91%)	149 (93%)	10 (6%)	1 (1%)	25	21
1	D	163/176 (93%)	153 (94%)	9 (6%)	1 (1%)	25	21
All	All	643/704 (91%)	597 (93%)	38 (6%)	8 (1%)	13	8

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	116	ILE
1	B	117	ILE
1	A	28	PRO
1	B	116	ILE
1	C	28	PRO

### 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	135/157 (86%)	129 (96%)	6 (4%)	28	28
1	B	132/157 (84%)	120 (91%)	12 (9%)	9	6
1	C	134/157 (85%)	129 (96%)	5 (4%)	34	35
1	D	141/157 (90%)	134 (95%)	7 (5%)	24	23
All	All	542/628 (86%)	512 (94%)	30 (6%)	21	19

5 of 30 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	103	LEU
1	B	118	ASP
1	D	88	GLU
1	B	116	ILE
1	B	122	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

179 ligands are modelled in this entry.

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	EDO	D	220	-	3,3,3	0.30	0	2,2,2	0.67	0
9	MOH	B	228	-	1,1,1	0.08	0	-		
8	EOH	C	224	-	2,2,2	0.39	0	1,1,1	0.38	0
5	EDO	B	207	-	3,3,3	0.53	0	2,2,2	1.23	0
15	P6G	D	209	-	18,18,18	0.55	0	17,17,17	0.80	1 (5%)
6	GOL	C	216	-	5,5,5	0.96	0	5,5,5	0.97	0
7	PDO	A	220	-	4,4,4	0.33	0	3,3,3	0.37	0
14	P33	C	207	-	21,21,21	0.48	0	20,20,20	0.31	0
7	PDO	B	214	-	4,4,4	0.41	0	3,3,3	0.95	0
5	EDO	A	209	-	3,3,3	0.46	0	2,2,2	0.34	0
5	EDO	A	217	-	3,3,3	0.46	0	2,2,2	0.34	0
8	EOH	A	227	-	2,2,2	0.39	0	1,1,1	0.38	0
4	PEG	A	207	-	6,6,6	0.53	0	5,5,5	2.06	2 (40%)
9	MOH	D	239	-	1,1,1	0.11	0	-		
9	MOH	A	242	-	1,1,1	0.06	0	-		
8	EOH	B	225	-	2,2,2	0.61	0	1,1,1	0.43	0
5	EDO	A	210	-	3,3,3	0.46	0	2,2,2	0.34	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
8	EOH	A	233	-	2,2,2	0.23	0	1,1,1	0.40	0
5	EDO	C	213	-	3,3,3	0.46	0	2,2,2	0.34	0
3	PG0	D	204	-	7,7,7	0.44	0	6,6,6	0.26	0
8	EOH	D	230	-	2,2,2	0.40	0	1,1,1	0.39	0
9	MOH	C	234	-	1,1,1	0.07	0	-		
5	EDO	D	218	-	3,3,3	1.21	1 (33%)	2,2,2	0.53	0
3	PG0	A	205	-	7,7,7	0.32	0	6,6,6	1.44	2 (33%)
7	PDO	B	213	-	4,4,4	0.33	0	3,3,3	0.37	0
13	PGE	B	233	-	9,9,9	0.44	0	8,8,8	0.29	0
8	EOH	A	237	-	2,2,2	0.70	0	1,1,1	0.73	0
5	EDO	C	211	-	3,3,3	0.46	0	2,2,2	0.34	0
8	EOH	D	226	-	2,2,2	0.40	0	1,1,1	0.38	0
9	MOH	C	233	-	1,1,1	0.08	0	-		
5	EDO	A	213	-	3,3,3	0.59	0	2,2,2	0.14	0
9	MOH	D	244	-	1,1,1	0.31	0	-		
12	ETE	C	208	-	13,13,13	0.66	0	12,12,12	1.37	3 (25%)
9	MOH	D	241	-	1,1,1	0.05	0	-		
5	EDO	C	209	-	3,3,3	1.16	0	2,2,2	1.39	0
8	EOH	D	228	-	2,2,2	0.40	0	1,1,1	0.39	0
7	PDO	A	222	-	4,4,4	0.32	0	3,3,3	0.37	0
7	PDO	D	224	-	4,4,4	0.32	0	3,3,3	0.37	0
9	MOH	C	232	-	1,1,1	0.20	0	-		
5	EDO	D	213	-	3,3,3	0.45	0	2,2,2	0.46	0
9	MOH	B	227	-	1,1,1	0.07	0	-		
9	MOH	C	237	-	1,1,1	0.12	0	-		
6	GOL	C	218	-	5,5,5	1.63	1 (20%)	5,5,5	2.37	2 (40%)
8	EOH	B	223	-	2,2,2	0.39	0	1,1,1	0.39	0
8	EOH	C	229	-	2,2,2	0.40	0	1,1,1	0.39	0
5	EDO	C	210	-	3,3,3	0.46	0	2,2,2	0.34	0
4	PEG	C	203	-	6,6,6	0.43	0	5,5,5	0.31	0
5	EDO	A	211	-	3,3,3	0.46	0	2,2,2	0.34	0
5	EDO	B	206	-	3,3,3	0.45	0	2,2,2	0.33	0
8	EOH	A	228	-	2,2,2	0.40	0	1,1,1	0.39	0
9	MOH	A	240	-	1,1,1	0.07	0	-		
3	PG0	D	203	-	7,7,7	0.44	0	6,6,6	0.27	0
8	EOH	B	226	-	2,2,2	0.37	0	1,1,1	0.17	0
9	MOH	A	244	-	1,1,1	0.08	0	-		
8	EOH	D	231	-	2,2,2	0.40	0	1,1,1	0.39	0
10	PGO	D	246	-	3,4,4	0.25	0	1,4,4	0.03	0
6	GOL	A	218	-	5,5,5	1.41	1 (20%)	5,5,5	2.62	3 (60%)
10	PGO	D	247	-	3,4,4	1.57	1 (33%)	1,4,4	0.95	0
13	PGE	C	240	-	9,9,9	0.45	0	8,8,8	0.29	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	PG0	C	202	-	7,7,7	0.74	0	6,6,6	0.84	0
7	PDO	C	221	-	4,4,4	0.32	0	3,3,3	0.37	0
9	MOH	A	245	-	1,1,1	0.07	0	-		
3	PG0	A	203	-	7,7,7	0.77	0	6,6,6	0.69	0
9	MOH	C	235	-	1,1,1	0.08	0	-		
9	MOH	D	237	-	1,1,1	0.07	0	-		
5	EDO	D	217	-	3,3,3	0.91	0	2,2,2	0.73	0
7	PDO	D	223	-	4,4,4	0.32	0	3,3,3	0.37	0
4	PEG	C	204	-	6,6,6	0.42	0	5,5,5	0.31	0
3	PG0	C	201	-	7,7,7	0.55	0	6,6,6	1.60	1 (16%)
5	EDO	A	214	-	3,3,3	0.39	0	2,2,2	0.84	0
11	ETX	D	250	-	5,5,5	0.64	0	4,4,4	0.82	0
6	GOL	C	217	-	5,5,5	1.29	1 (20%)	5,5,5	1.31	1 (20%)
9	MOH	A	246	-	1,1,1	0.07	0	-		
5	EDO	B	211	-	3,3,3	0.84	0	2,2,2	0.40	0
5	EDO	D	215	-	3,3,3	0.46	0	2,2,2	0.34	0
7	PDO	A	225	-	4,4,4	0.94	0	3,3,3	0.81	0
9	MOH	A	239	-	1,1,1	0.07	0	-		
2	PG4	A	202	-	12,12,12	0.58	0	11,11,11	1.25	3 (27%)
11	ETX	B	236	-	5,5,5	0.53	0	4,4,4	1.21	1 (25%)
5	EDO	D	221	-	3,3,3	0.46	0	2,2,2	0.34	0
15	P6G	D	210	-	18,18,18	0.82	0	17,17,17	1.65	4 (23%)
8	EOH	C	223	-	2,2,2	0.39	0	1,1,1	0.38	0
8	EOH	C	230	-	2,2,2	0.39	0	1,1,1	0.39	0
3	PG0	A	204	-	7,7,7	0.45	0	6,6,6	0.27	0
10	PGO	B	231	-	3,4,4	0.25	0	1,4,4	0.02	0
8	EOH	A	226	-	2,2,2	0.05	0	1,1,1	0.13	0
9	MOH	D	240	-	1,1,1	0.07	0	-		
8	EOH	B	222	-	2,2,2	0.39	0	1,1,1	0.38	0
10	PGO	A	249	-	3,4,4	0.54	0	1,4,4	0.19	0
8	EOH	C	227	-	2,2,2	0.39	0	1,1,1	0.38	0
9	MOH	A	241	-	1,1,1	0.07	0	-		
8	EOH	D	229	-	2,2,2	0.39	0	1,1,1	0.38	0
6	GOL	D	222	-	5,5,5	1.52	1 (20%)	5,5,5	0.78	0
8	EOH	A	238	-	2,2,2	0.17	0	1,1,1	0.28	0
9	MOH	D	242	-	1,1,1	0.07	0	-		
9	MOH	C	236	-	1,1,1	0.01	0	-		
13	PGE	C	241	-	9,9,9	1.26	2 (22%)	8,8,8	2.12	2 (25%)
8	EOH	B	215	-	2,2,2	0.39	0	1,1,1	0.38	0
8	EOH	B	220	-	2,2,2	0.39	0	1,1,1	0.38	0
5	EDO	D	212	-	3,3,3	0.43	0	2,2,2	0.48	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
8	EOH	B	221	-	2,2,2	0.40	0	1,1,1	0.65	0
5	EDO	D	211	-	3,3,3	0.49	0	2,2,2	0.34	0
4	PEG	D	207	-	6,6,6	0.47	0	5,5,5	0.92	0
8	EOH	A	236	-	2,2,2	0.55	0	1,1,1	0.13	0
5	EDO	D	214	-	3,3,3	0.58	0	2,2,2	0.46	0
8	EOH	B	219	-	2,2,2	0.39	0	1,1,1	0.38	0
7	PDO	A	219	-	4,4,4	0.58	0	3,3,3	2.03	1 (33%)
8	EOH	D	234	-	2,2,2	0.54	0	1,1,1	0.27	0
8	EOH	C	226	-	2,2,2	0.49	0	1,1,1	0.38	0
11	ETX	C	242	-	5,5,5	0.44	0	4,4,4	0.29	0
9	MOH	D	243	-	1,1,1	0.07	0	-		
8	EOH	A	235	-	2,2,2	0.39	0	1,1,1	0.39	0
5	EDO	D	216	-	3,3,3	0.46	0	2,2,2	0.34	0
5	EDO	A	216	-	3,3,3	0.80	0	2,2,2	0.80	0
5	EDO	C	212	-	3,3,3	0.45	0	2,2,2	0.34	0
5	EDO	B	210	-	3,3,3	0.71	0	2,2,2	1.02	0
2	PG4	B	201	-	12,12,12	0.95	0	11,11,11	1.42	1 (9%)
11	ETX	B	235	-	5,5,5	0.44	0	4,4,4	0.29	0
2	PG4	A	201	-	12,12,12	0.54	0	11,11,11	0.46	0
8	EOH	A	232	-	2,2,2	0.63	0	1,1,1	0.85	0
11	ETX	B	234	-	5,5,5	0.33	0	4,4,4	0.79	0
7	PDO	A	221	-	4,4,4	0.33	0	3,3,3	0.37	0
8	EOH	D	235	-	2,2,2	0.57	0	1,1,1	0.84	0
10	PGO	D	245	-	3,4,4	1.12	0	1,4,4	2.44	1 (100%)
7	PDO	A	224	-	4,4,4	0.33	0	3,3,3	0.37	0
9	MOH	A	243	-	1,1,1	0.12	0	-		
8	EOH	D	227	-	2,2,2	0.40	0	1,1,1	0.39	0
8	EOH	A	234	-	2,2,2	0.40	0	1,1,1	0.39	0
5	EDO	D	219	-	3,3,3	0.46	0	2,2,2	0.34	0
8	EOH	D	233	-	2,2,2	0.39	0	1,1,1	0.38	0
4	PEG	D	205	-	6,6,6	0.43	0	5,5,5	0.31	0
4	PEG	C	206	-	6,6,6	0.60	0	5,5,5	1.25	0
8	EOH	B	224	-	2,2,2	0.48	0	1,1,1	0.42	0
8	EOH	B	217	-	2,2,2	0.39	0	1,1,1	0.38	0
8	EOH	C	225	-	2,2,2	0.40	0	1,1,1	0.39	0
8	EOH	D	225	-	2,2,2	0.44	0	1,1,1	0.28	0
4	PEG	C	205	-	6,6,6	0.66	0	5,5,5	2.42	3 (60%)
12	ETE	B	205	-	13,13,13	0.70	0	12,12,12	1.48	2 (16%)
8	EOH	C	228	-	2,2,2	0.39	0	1,1,1	0.38	0
4	PEG	A	208	-	6,6,6	0.60	0	5,5,5	1.13	1 (20%)
8	EOH	C	222	-	2,2,2	0.39	0	1,1,1	0.38	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
11	ETX	A	251	-	5,5,5	0.81	0	4,4,4	1.62	1 (25%)
5	EDO	B	209	-	3,3,3	0.48	0	2,2,2	0.22	0
4	PEG	B	204	-	6,6,6	0.30	0	5,5,5	1.34	1 (20%)
9	MOH	B	229	-	1,1,1	0.06	0	-		
10	PGO	C	238	-	3,4,4	1.32	0	1,4,4	0.72	0
8	EOH	A	229	-	2,2,2	0.20	0	1,1,1	0.56	0
13	PGE	D	248	-	9,9,9	0.44	0	8,8,8	0.29	0
5	EDO	A	215	-	3,3,3	0.45	0	2,2,2	0.34	0
2	PG4	D	202	-	12,12,12	0.45	0	11,11,11	0.28	0
3	PG0	A	206	-	7,7,7	1.07	1 (14%)	6,6,6	1.92	3 (50%)
3	PG0	B	202	-	7,7,7	0.44	0	6,6,6	0.27	0
9	MOH	D	238	-	1,1,1	0.08	0	-		
8	EOH	D	236	-	2,2,2	0.39	0	1,1,1	0.38	0
13	PGE	C	239	-	9,9,9	0.44	0	8,8,8	0.29	0
5	EDO	B	208	-	3,3,3	0.36	0	2,2,2	0.25	0
10	PGO	A	248	-	3,4,4	0.45	0	1,4,4	0.48	0
11	ETX	A	250	-	5,5,5	0.44	0	4,4,4	0.29	0
7	PDO	A	223	-	4,4,4	0.32	0	3,3,3	0.37	0
10	PGO	B	232	-	3,4,4	0.31	0	1,4,4	1.18	0
11	ETX	D	249	-	5,5,5	0.41	0	4,4,4	0.56	0
8	EOH	B	216	-	2,2,2	0.40	0	1,1,1	0.38	0
5	EDO	C	215	-	3,3,3	1.44	1 (33%)	2,2,2	0.40	0
10	PGO	B	230	-	3,4,4	3.20	1 (33%)	1,4,4	2.01	1 (100%)
4	PEG	D	206	-	6,6,6	0.43	0	5,5,5	0.31	0
2	PG4	D	201	-	12,12,12	1.33	2 (16%)	11,11,11	1.64	2 (18%)
5	EDO	A	212	-	3,3,3	0.46	0	2,2,2	0.34	0
4	PEG	B	203	-	6,6,6	0.43	0	5,5,5	0.31	0
10	PGO	A	247	-	3,4,4	0.65	0	1,4,4	1.44	0
8	EOH	B	218	-	2,2,2	0.40	0	1,1,1	0.38	0
8	EOH	A	230	-	2,2,2	0.40	0	1,1,1	0.39	0
5	EDO	C	214	-	3,3,3	1.00	0	2,2,2	1.16	0
8	EOH	A	231	-	2,2,2	0.40	0	1,1,1	0.38	0
7	PDO	C	220	-	4,4,4	0.32	0	3,3,3	0.37	0
8	EOH	D	232	-	2,2,2	0.39	0	1,1,1	0.38	0
7	PDO	B	212	-	4,4,4	0.32	0	3,3,3	0.37	0
15	P6G	D	208	-	18,18,18	0.46	0	17,17,17	0.27	0
6	GOL	C	219	-	5,5,5	1.15	0	5,5,5	2.21	3 (60%)
8	EOH	C	231	-	2,2,2	0.39	0	1,1,1	0.38	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	EDO	D	220	-	-	1/1/1/1	-
5	EDO	B	207	-	-	1/1/1/1	-
15	P6G	D	209	-	-	7/16/16/16	-
6	GOL	C	216	-	-	2/4/4/4	-
11	ETX	B	236	-	-	2/3/3/3	-
14	P33	C	207	-	-	11/19/19/19	-
7	PDO	B	214	-	-	1/2/2/2	-
5	EDO	A	209	-	-	0/1/1/1	-
5	EDO	A	217	-	-	1/1/1/1	-
4	PEG	A	207	-	-	3/4/4/4	-
5	EDO	C	213	-	-	1/1/1/1	-
3	PG0	D	204	-	-	3/5/5/5	-
5	EDO	D	218	-	-	1/1/1/1	-
3	PG0	A	205	-	-	3/5/5/5	-
7	PDO	B	213	-	-	1/2/2/2	-
13	PGE	B	233	-	-	3/7/7/7	-
5	EDO	C	211	-	-	1/1/1/1	-
5	EDO	A	213	-	-	1/1/1/1	-
10	PGO	C	238	-	-	0/2/2/2	-
12	ETE	C	208	-	-	6/11/11/11	-
7	PDO	A	222	-	-	2/2/2/2	-
7	PDO	D	224	-	-	1/2/2/2	-
5	EDO	D	213	-	-	0/1/1/1	-
6	GOL	C	218	-	-	4/4/4/4	-
5	EDO	C	210	-	-	1/1/1/1	-
4	PEG	C	203	-	-	1/4/4/4	-
5	EDO	A	211	-	-	1/1/1/1	-
5	EDO	B	206	-	-	1/1/1/1	-
5	EDO	D	219	-	-	1/1/1/1	-
11	ETX	D	249	-	-	2/3/3/3	-
10	PGO	D	246	-	-	0/2/2/2	-
6	GOL	A	218	-	-	4/4/4/4	-
10	PGO	D	247	-	-	2/2/2/2	-
13	PGE	C	240	-	-	3/7/7/7	-
3	PG0	C	202	-	-	4/5/5/5	-
7	PDO	C	221	-	-	1/2/2/2	-
3	PG0	A	203	-	-	3/5/5/5	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	D	217	-	-	0/1/1/1	-
7	PDO	D	223	-	-	1/2/2/2	-
4	PEG	C	204	-	-	3/4/4/4	-
3	PG0	C	201	-	-	1/5/5/5	-
5	EDO	A	214	-	-	1/1/1/1	-
11	ETX	D	250	-	-	2/3/3/3	-
6	GOL	C	217	-	-	4/4/4/4	-
5	EDO	B	211	-	-	0/1/1/1	-
5	EDO	D	215	-	-	1/1/1/1	-
7	PDO	A	225	-	-	1/2/2/2	-
2	PG4	A	202	-	-	6/10/10/10	-
5	EDO	D	221	-	-	1/1/1/1	-
3	PG0	A	204	-	-	4/5/5/5	-
10	PGO	B	231	-	-	2/2/2/2	-
13	PGE	C	239	-	-	4/7/7/7	-
10	PGO	A	249	-	-	2/2/2/2	-
5	EDO	A	210	-	-	1/1/1/1	-
6	GOL	D	222	-	-	4/4/4/4	-
13	PGE	C	241	-	-	4/7/7/7	-
5	EDO	D	212	-	-	1/1/1/1	-
5	EDO	D	211	-	-	1/1/1/1	-
4	PEG	D	207	-	-	3/4/4/4	-
5	EDO	D	214	-	-	0/1/1/1	-
7	PDO	A	219	-	-	1/2/2/2	-
15	P6G	D	210	-	-	9/16/16/16	-
11	ETX	C	242	-	-	3/3/3/3	-
5	EDO	D	216	-	-	1/1/1/1	-
5	EDO	A	216	-	-	1/1/1/1	-
5	EDO	C	212	-	-	1/1/1/1	-
5	EDO	B	210	-	-	0/1/1/1	-
2	PG4	B	201	-	-	6/10/10/10	-
11	ETX	B	235	-	-	1/3/3/3	-
2	PG4	A	201	-	-	4/10/10/10	-
7	PDO	A	224	-	-	2/2/2/2	-
11	ETX	B	234	-	-	2/3/3/3	-
7	PDO	A	221	-	-	1/2/2/2	-
10	PGO	D	245	-	-	2/2/2/2	-
13	PGE	D	248	-	-	6/7/7/7	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PG0	D	203	-	-	1/5/5/5	-
4	PEG	D	205	-	-	2/4/4/4	-
4	PEG	C	206	-	-	2/4/4/4	-
4	PEG	C	205	-	-	3/4/4/4	-
12	ETE	B	205	-	-	6/11/11/11	-
4	PEG	A	208	-	-	3/4/4/4	-
11	ETX	A	251	-	-	2/3/3/3	-
5	EDO	B	209	-	-	1/1/1/1	-
4	PEG	B	204	-	-	2/4/4/4	-
5	EDO	A	215	-	-	0/1/1/1	-
2	PG4	D	202	-	-	2/10/10/10	-
3	PG0	A	206	-	-	2/5/5/5	-
3	PG0	B	202	-	-	1/5/5/5	-
5	EDO	B	208	-	-	1/1/1/1	-
10	PGO	A	248	-	-	2/2/2/2	-
7	PDO	A	220	-	-	1/2/2/2	-
11	ETX	A	250	-	-	2/3/3/3	-
7	PDO	A	223	-	-	1/2/2/2	-
10	PGO	B	232	-	-	2/2/2/2	-
5	EDO	C	215	-	-	1/1/1/1	-
10	PGO	B	230	-	1/1/1/1	1/2/2/2	-
4	PEG	D	206	-	-	4/4/4/4	-
2	PG4	D	201	-	-	6/10/10/10	-
5	EDO	A	212	-	-	0/1/1/1	-
4	PEG	B	203	-	-	3/4/4/4	-
10	PGO	A	247	-	-	2/2/2/2	-
5	EDO	C	214	-	-	0/1/1/1	-
7	PDO	C	220	-	-	2/2/2/2	-
5	EDO	C	209	-	-	1/1/1/1	-
7	PDO	B	212	-	-	1/2/2/2	-
15	P6G	D	208	-	-	9/16/16/16	-
6	GOL	C	219	-	-	4/4/4/4	-

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	B	230	PGO	O2-C2	-5.54	1.19	1.43
6	C	218	GOL	O2-C2	-3.07	1.34	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	222	GOL	O2-C2	-2.84	1.34	1.43
6	A	218	GOL	O2-C2	-2.82	1.35	1.43
2	D	201	PG4	O4-C6	-2.34	1.31	1.42

The worst 5 of 45 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	C	241	PGE	C3-O2-C2	-4.33	94.52	113.29
6	C	218	GOL	O2-C2-C3	-4.04	91.34	109.12
15	D	210	P6G	O7-C6-C5	3.94	128.18	110.39
4	A	207	PEG	O2-C2-C1	3.78	126.65	110.07
6	A	218	GOL	O1-C1-C2	3.53	127.11	110.20

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
10	B	230	PGO	C2

5 of 237 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	C	216	GOL	C1-C2-C3-O3
6	C	216	GOL	O2-C2-C3-O3
7	B	214	PDO	O1-C1-C2-C3
7	A	222	PDO	O1-C1-C2-C3
7	D	224	PDO	O1-C1-C2-C3

There are no ring outliers.

85 monomers are involved in 213 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	220	EDO	1	0
8	C	224	EOH	1	0
5	B	207	EDO	3	0
15	D	209	P6G	15	0
7	A	220	PDO	2	0
14	C	207	P33	14	0
5	A	209	EDO	2	0
4	A	207	PEG	4	0
9	D	239	MOH	1	0
5	A	210	EDO	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	204	PG0	5	0
8	D	230	EOH	11	0
3	A	205	PG0	1	0
13	B	233	PGE	3	0
12	C	208	ETE	1	0
5	C	209	EDO	1	0
7	A	222	PDO	1	0
7	D	224	PDO	11	0
8	B	223	EOH	2	0
5	C	210	EDO	1	0
4	C	203	PEG	8	0
5	B	206	EDO	1	0
3	D	203	PG0	4	0
8	B	226	EOH	1	0
10	D	246	PGO	5	0
13	C	240	PGE	1	0
3	C	202	PG0	5	0
7	C	221	PDO	1	0
3	A	203	PG0	3	0
9	D	237	MOH	1	0
4	C	204	PEG	1	0
3	C	201	PG0	3	0
5	A	214	EDO	1	0
11	D	250	ETX	6	0
6	C	217	GOL	1	0
2	A	202	PG4	1	0
11	B	236	ETX	1	0
15	D	210	P6G	5	0
3	A	204	PG0	7	0
8	A	226	EOH	2	0
10	A	249	PGO	1	0
8	C	227	EOH	1	0
6	D	222	GOL	2	0
13	C	241	PGE	2	0
8	B	220	EOH	2	0
5	D	212	EDO	2	0
8	A	236	EOH	2	0
7	A	219	PDO	3	0
8	C	226	EOH	3	0
5	A	216	EDO	2	0
5	C	212	EDO	2	0
2	B	201	PG4	2	0

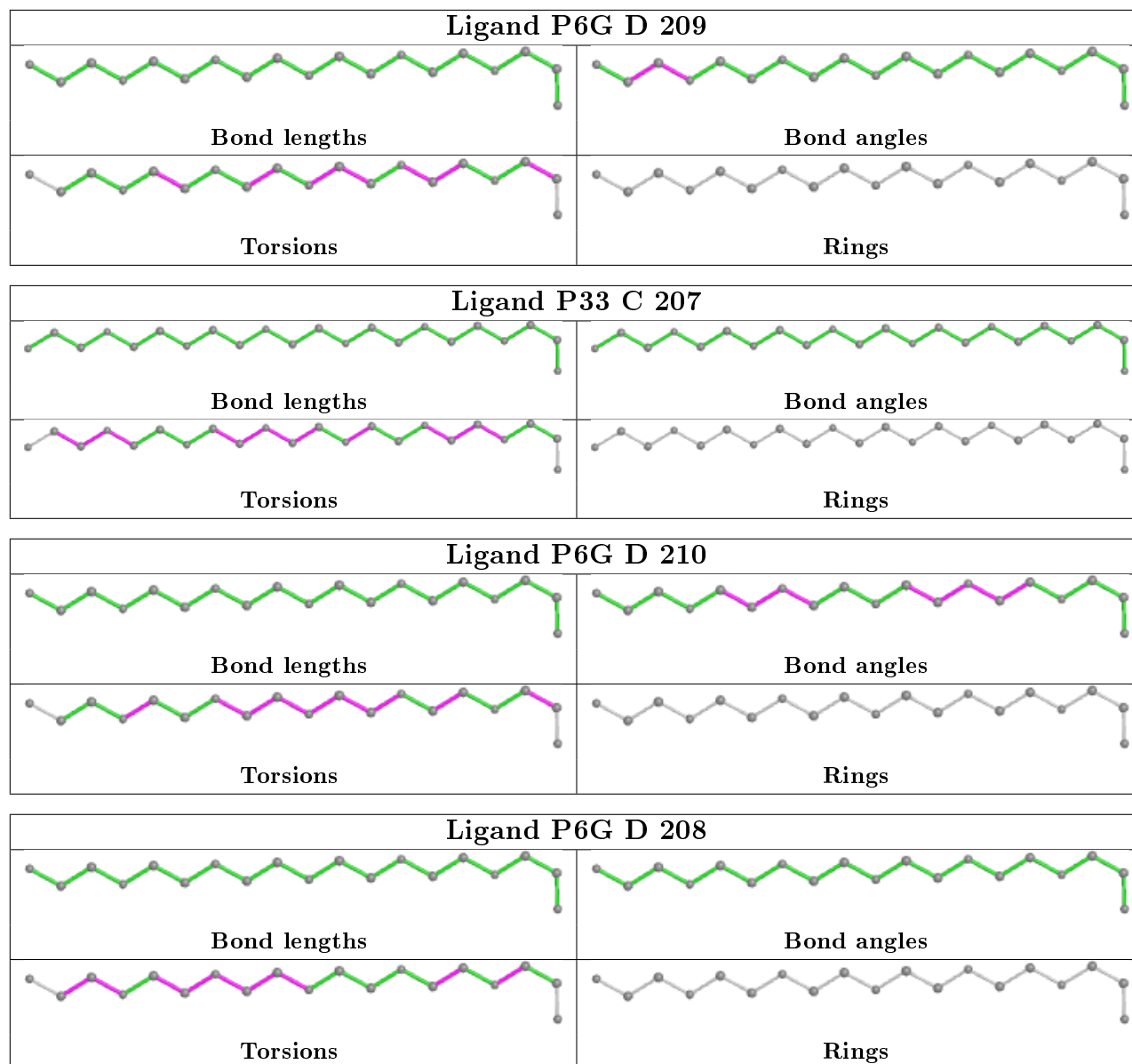
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	232	EOH	1	0
11	B	234	ETX	2	0
7	A	221	PDO	7	0
10	D	245	PGO	4	0
4	D	205	PEG	6	0
8	B	217	EOH	2	0
8	C	225	EOH	4	0
8	D	225	EOH	1	0
4	C	205	PEG	4	0
12	B	205	ETE	4	0
8	C	222	EOH	1	0
5	B	209	EDO	1	0
9	B	229	MOH	2	0
13	D	248	PGE	1	0
2	D	202	PG4	9	0
3	A	206	PG0	5	0
3	B	202	PG0	2	0
13	C	239	PGE	5	0
11	A	250	ETX	8	0
11	D	249	ETX	12	0
5	C	215	EDO	1	0
10	B	230	PGO	2	0
4	D	206	PEG	6	0
2	D	201	PG4	4	0
5	A	212	EDO	1	0
10	A	247	PGO	10	0
8	A	230	EOH	1	0
5	C	214	EDO	1	0
8	A	231	EOH	1	0
7	B	212	PDO	1	0
15	D	208	P6G	2	0
6	C	219	GOL	1	0
8	C	231	EOH	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	165/176 (93%)	0.58	17 (10%) 6 8	23, 38, 71, 84	0
1	B	161/176 (91%)	0.40	10 (6%) 20 25	22, 38, 62, 76	0
1	C	161/176 (91%)	0.38	10 (6%) 20 25	21, 33, 56, 83	0
1	D	166/176 (94%)	0.48	12 (7%) 15 19	21, 36, 63, 91	0
All	All	653/704 (92%)	0.46	49 (7%) 14 18	21, 37, 64, 91	0

The worst 5 of 49 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	29	THR	8.8
1	A	2	ALA	6.8
1	A	32	THR	6.4
1	A	29	THR	5.3
1	A	28	PRO	5.2

### 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 carbohydrates 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<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( $\text{\AA}^2$ )	Q<0.9
8	EOH	D	230	3/3	0.26	0.24	57,57,60,62	0
6	GOL	C	216	6/6	0.41	0.55	59,64,71,72	0
8	EOH	A	227	3/3	0.44	0.29	48,48,62,67	0
11	ETX	C	242	6/6	0.45	0.59	52,63,63,70	0
9	MOH	D	239	2/2	0.47	0.29	62,62,62,62	0
15	P6G	D	210	19/19	0.49	0.38	56,71,87,88	0
4	PEG	C	206	7/7	0.50	0.26	50,55,61,66	0
10	PGO	D	246	5/5	0.53	0.26	54,55,59,60	0
13	PGE	C	239	10/10	0.55	0.24	68,71,76,76	0
5	EDO	B	209	4/4	0.56	0.51	63,64,64,65	0
11	ETX	B	236	6/6	0.57	0.44	61,64,70,73	0
3	PG0	A	205	8/8	0.57	0.32	55,61,65,70	0
5	EDO	D	220	4/4	0.58	0.80	68,68,72,73	0
9	MOH	A	243	2/2	0.59	0.44	65,65,65,67	0
5	EDO	B	210	4/4	0.59	0.24	75,76,77,80	0
3	PG0	A	206	8/8	0.60	0.32	64,68,72,73	0
9	MOH	A	244	2/2	0.60	0.29	62,62,62,70	0
11	ETX	D	250	6/6	0.61	0.26	58,62,65,66	0
12	ETE	C	208	14/14	0.61	0.25	56,69,75,80	0
8	EOH	A	233	3/3	0.61	0.28	50,50,54,57	0
5	EDO	B	207	4/4	0.61	0.27	56,61,61,67	0
6	GOL	C	219	6/6	0.61	0.32	66,71,74,78	0
4	PEG	B	204	7/7	0.62	0.38	61,67,74,76	0
2	PG4	A	202	13/13	0.62	0.34	52,61,76,77	0
4	PEG	A	207	7/7	0.63	0.22	63,70,73,74	0
9	MOH	D	243	2/2	0.64	0.23	56,56,56,58	0
10	PGO	A	249	5/5	0.64	0.29	42,44,48,48	0
8	EOH	C	224	3/3	0.64	0.20	57,57,59,63	0
9	MOH	C	234	2/2	0.65	0.20	46,46,46,49	0
8	EOH	B	221	3/3	0.65	0.18	67,67,71,73	0
12	ETE	B	205	14/14	0.66	0.22	61,69,76,77	0
11	ETX	A	250	6/6	0.66	0.34	63,74,75,78	0
5	EDO	D	221	4/4	0.66	0.27	70,70,75,77	0
9	MOH	A	241	2/2	0.67	0.33	34,34,34,41	0
13	PGE	C	240	10/10	0.67	0.39	56,71,77,83	0
3	PG0	A	204	8/8	0.68	0.27	36,49,55,58	0
9	MOH	C	232	2/2	0.68	0.24	45,45,45,48	0
7	PDO	A	225	5/5	0.68	0.27	48,54,56,61	0
8	EOH	C	230	3/3	0.68	0.43	68,68,70,74	0
15	P6G	D	209	19/19	0.69	0.40	79,90,96,97	0
3	PG0	C	202	8/8	0.69	0.27	49,59,62,68	0
6	GOL	D	222	6/6	0.69	0.35	56,58,65,65	0
9	MOH	C	236	2/2	0.69	0.29	50,50,50,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	PG0	D	204	8/8	0.69	0.32	42,49,57,66	0
7	PDO	A	223	5/5	0.69	0.18	44,45,50,57	0
4	PEG	D	207	7/7	0.69	0.32	62,75,81,84	0
8	EOH	B	226	3/3	0.70	0.29	64,64,70,71	0
7	PDO	A	224	5/5	0.70	0.34	70,71,72,72	0
3	PG0	D	203	8/8	0.71	0.34	57,62,63,64	0
7	PDO	A	219	5/5	0.71	0.34	68,70,76,77	0
2	PG4	A	201	13/13	0.71	0.31	55,63,68,69	0
10	PGO	D	245	5/5	0.71	0.39	49,51,54,66	0
8	EOH	A	238	3/3	0.71	0.30	60,60,62,65	0
8	EOH	A	229	3/3	0.72	0.23	59,59,68,71	0
4	PEG	C	205	7/7	0.72	0.18	55,59,62,67	0
9	MOH	B	227	2/2	0.73	0.23	45,45,45,45	0
3	PG0	B	202	8/8	0.73	0.25	43,57,59,64	0
5	EDO	D	214	4/4	0.73	0.26	50,51,54,54	0
14	P33	C	207	22/22	0.74	0.37	44,59,74,77	0
8	EOH	A	228	3/3	0.74	0.26	58,58,61,64	0
10	PGO	A	248	5/5	0.74	0.23	49,50,57,58	0
8	EOH	D	235	3/3	0.74	0.25	46,46,46,51	0
9	MOH	D	244	2/2	0.74	0.25	44,44,44,47	0
4	PEG	D	206	7/7	0.74	0.48	30,39,50,51	0
4	PEG	B	203	7/7	0.74	0.20	56,60,63,64	0
8	EOH	C	226	3/3	0.74	0.37	55,55,56,58	0
5	EDO	D	219	4/4	0.75	0.28	73,75,77,88	0
9	MOH	D	241	2/2	0.75	0.23	60,60,60,63	0
5	EDO	A	212	4/4	0.75	0.25	55,58,60,62	0
13	PGE	D	248	10/10	0.75	0.29	54,65,76,79	0
7	PDO	B	214	5/5	0.75	0.22	50,54,65,75	0
7	PDO	B	213	5/5	0.76	0.24	60,64,70,71	0
8	EOH	A	237	3/3	0.76	0.23	64,64,66,70	0
4	PEG	A	208	7/7	0.76	0.19	68,73,78,81	0
5	EDO	D	218	4/4	0.76	0.32	50,56,60,67	0
4	PEG	D	205	7/7	0.76	0.24	38,45,52,52	0
10	PGO	A	247	5/5	0.76	0.18	62,65,69,77	0
5	EDO	A	217	4/4	0.76	0.20	70,74,74,79	0
5	EDO	B	211	4/4	0.77	0.24	47,52,52,52	0
9	MOH	B	229	2/2	0.77	0.20	65,65,65,65	0
8	EOH	D	232	3/3	0.77	0.28	49,49,53,53	0
5	EDO	A	211	4/4	0.77	0.21	67,70,71,73	0
11	ETX	B	234	6/6	0.78	0.30	55,62,69,73	0
8	EOH	A	226	3/3	0.78	0.20	49,49,52,55	0
8	EOH	C	225	3/3	0.78	0.17	50,50,54,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
11	ETX	D	249	6/6	0.78	0.17	60,64,67,70	0
5	EDO	C	213	4/4	0.78	0.20	58,58,59,60	0
3	PG0	A	203	8/8	0.78	0.26	45,50,60,63	0
5	EDO	D	217	4/4	0.78	0.40	41,42,43,43	0
11	ETX	A	251	6/6	0.78	0.17	59,71,74,78	0
3	PG0	C	201	8/8	0.78	0.20	47,51,58,59	0
5	EDO	B	208	4/4	0.78	0.24	56,58,62,62	0
5	EDO	A	213	4/4	0.79	0.51	54,55,57,61	0
7	PDO	D	223	5/5	0.79	0.22	40,41,45,48	0
4	PEG	C	204	7/7	0.79	0.19	30,32,36,37	0
5	EDO	D	216	4/4	0.79	0.41	44,47,51,54	0
13	PGE	B	233	10/10	0.79	0.34	56,63,69,84	0
8	EOH	C	228	3/3	0.79	0.29	49,49,52,55	0
10	PGO	B	231	5/5	0.79	0.17	51,60,64,65	0
9	MOH	C	237	2/2	0.80	0.22	51,51,51,55	0
7	PDO	C	221	5/5	0.80	0.20	29,34,40,40	0
6	GOL	C	218	6/6	0.80	0.29	53,57,63,66	0
5	EDO	D	213	4/4	0.80	0.18	47,51,51,58	0
10	PGO	D	247	5/5	0.80	0.19	40,44,49,52	0
7	PDO	B	212	5/5	0.80	0.18	40,46,49,51	0
8	EOH	B	225	3/3	0.80	0.22	48,48,49,57	0
8	EOH	D	233	3/3	0.81	0.23	48,48,51,51	0
8	EOH	B	220	3/3	0.81	0.39	54,54,58,59	0
5	EDO	B	206	4/4	0.81	0.28	36,40,42,42	0
7	PDO	C	220	5/5	0.81	0.19	53,55,59,60	0
7	PDO	A	220	5/5	0.81	0.22	46,51,54,55	0
8	EOH	A	232	3/3	0.81	0.19	55,55,67,69	0
5	EDO	A	214	4/4	0.81	0.19	63,69,72,73	0
8	EOH	A	236	3/3	0.82	0.50	41,41,45,47	0
7	PDO	A	222	5/5	0.82	0.19	55,56,60,66	0
5	EDO	A	216	4/4	0.82	0.14	47,51,52,56	0
9	MOH	B	228	2/2	0.82	0.19	47,47,47,54	0
5	EDO	C	214	4/4	0.82	0.24	52,56,56,56	0
2	PG4	B	201	13/13	0.82	0.15	54,58,63,66	0
5	EDO	D	215	4/4	0.82	0.19	44,46,50,51	0
8	EOH	B	223	3/3	0.82	0.27	46,46,49,57	0
5	EDO	A	215	4/4	0.82	0.26	54,55,56,65	0
8	EOH	A	230	3/3	0.83	0.19	65,65,72,80	0
11	ETX	B	235	6/6	0.83	0.16	45,55,56,61	0
5	EDO	A	210	4/4	0.83	0.17	43,46,46,52	0
6	GOL	A	218	6/6	0.83	0.18	48,50,53,66	0
10	PGO	B	230	5/5	0.83	0.16	30,35,41,45	0

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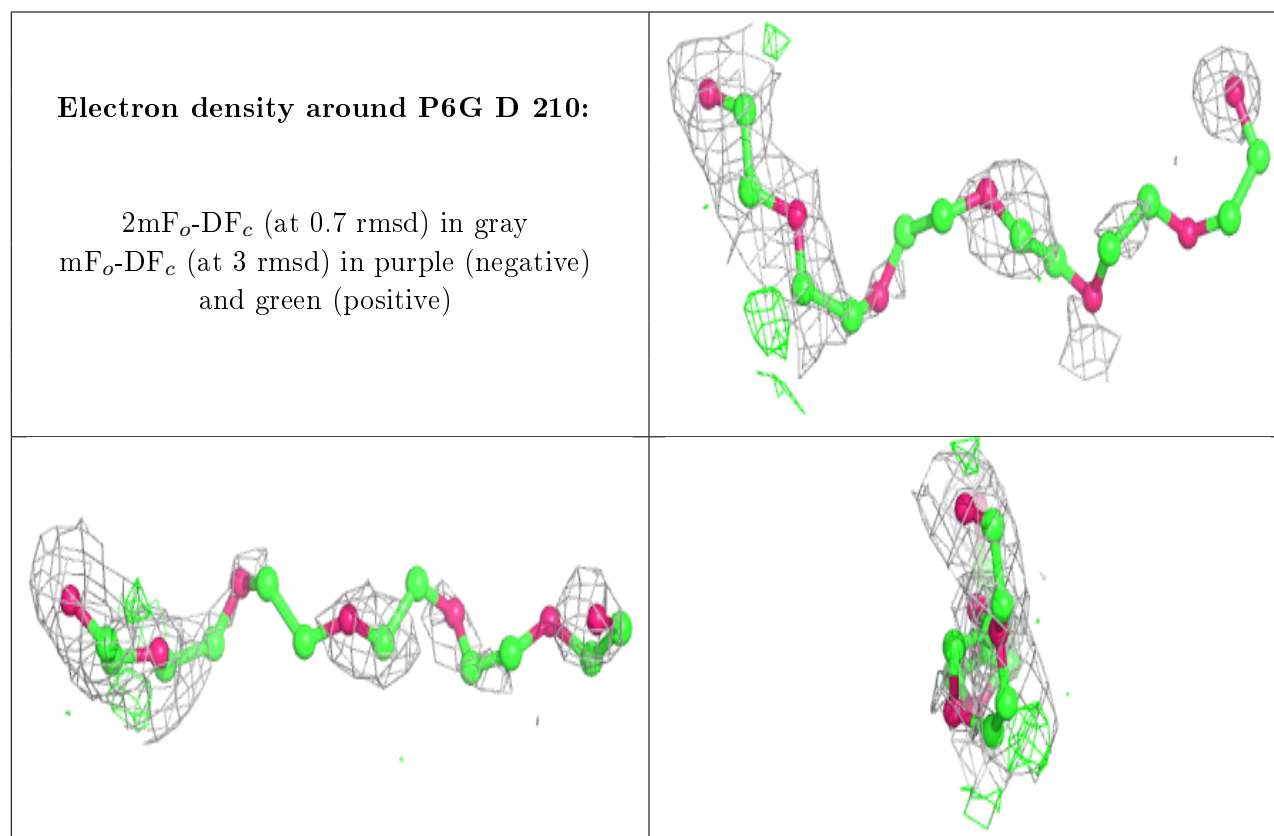
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
8	EOH	B	218	3/3	0.83	0.18	52,52,55,56	0
9	MOH	C	233	2/2	0.84	0.24	39,39,39,44	0
9	MOH	A	245	2/2	0.84	0.20	55,55,55,60	0
8	EOH	B	222	3/3	0.84	0.31	55,55,59,68	0
5	EDO	C	209	4/4	0.84	0.29	52,57,57,61	0
9	MOH	A	239	2/2	0.84	0.23	40,40,40,42	0
2	PG4	D	202	13/13	0.84	0.34	30,42,48,53	0
8	EOH	D	229	3/3	0.84	0.19	32,32,32,44	0
8	EOH	B	216	3/3	0.84	0.31	53,53,56,58	0
9	MOH	A	246	2/2	0.84	0.25	55,55,55,68	0
15	P6G	D	208	19/19	0.84	0.16	27,47,51,61	0
2	PG4	D	201	13/13	0.84	0.28	41,47,52,56	0
9	MOH	C	235	2/2	0.85	0.24	63,63,63,65	0
8	EOH	C	229	3/3	0.85	0.24	49,49,58,59	0
6	GOL	C	217	6/6	0.85	0.22	42,47,51,59	0
5	EDO	C	211	4/4	0.85	0.15	62,70,70,74	0
5	EDO	A	209	4/4	0.85	0.20	51,55,55,60	0
9	MOH	D	238	2/2	0.85	0.13	51,51,51,56	0
8	EOH	B	215	3/3	0.85	0.15	59,59,59,69	0
10	PGO	C	238	5/5	0.85	0.16	40,44,52,53	0
8	EOH	D	228	3/3	0.85	0.28	41,41,48,51	0
5	EDO	C	210	4/4	0.86	0.20	37,45,45,46	0
13	PGE	C	241	10/10	0.86	0.24	38,51,59,63	0
8	EOH	C	222	3/3	0.86	0.20	55,55,55,59	0
4	PEG	C	203	7/7	0.86	0.49	35,39,44,50	0
8	EOH	C	227	3/3	0.86	0.15	53,53,54,61	0
7	PDO	A	221	5/5	0.86	0.25	35,35,38,50	0
8	EOH	D	234	3/3	0.86	0.25	45,45,48,56	0
10	PGO	B	232	5/5	0.86	0.13	44,50,60,61	0
8	EOH	A	231	3/3	0.87	0.12	59,59,63,63	0
8	EOH	A	234	3/3	0.87	0.29	50,50,51,61	0
7	PDO	D	224	5/5	0.87	0.25	21,26,32,35	0
8	EOH	B	224	3/3	0.88	0.25	54,54,58,61	0
9	MOH	A	242	2/2	0.88	0.22	29,29,29,34	0
5	EDO	C	212	4/4	0.89	0.26	48,51,57,58	0
8	EOH	D	227	3/3	0.89	0.17	46,46,51,63	0
5	EDO	C	215	4/4	0.89	0.19	38,48,51,54	0
8	EOH	B	217	3/3	0.90	0.24	30,30,36,42	0
9	MOH	D	242	2/2	0.90	0.26	45,45,45,48	0
8	EOH	B	219	3/3	0.90	0.11	39,39,46,56	0
5	EDO	D	211	4/4	0.91	0.20	40,42,47,59	0
9	MOH	D	237	2/2	0.91	0.47	35,35,35,41	0

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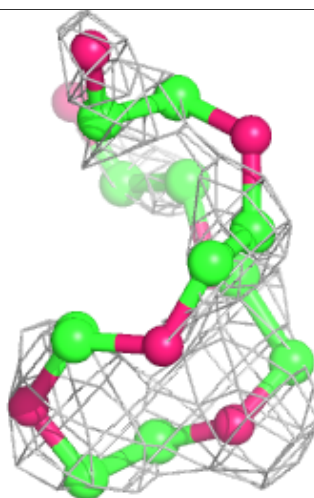
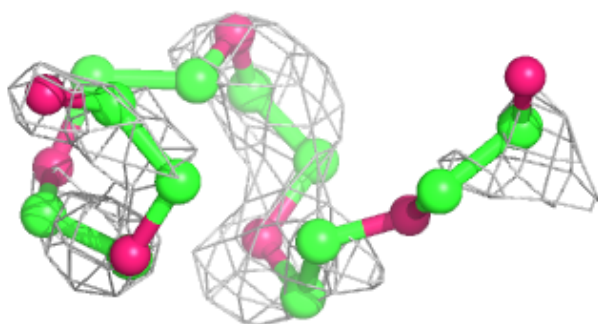
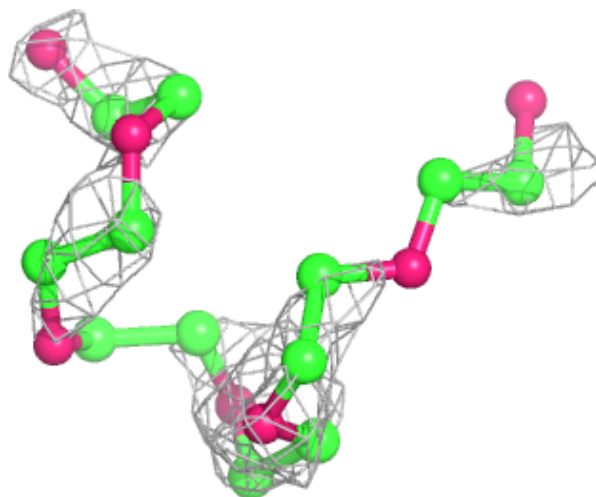
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
8	EOH	C	223	3/3	0.91	0.19	42,42,44,50	0
5	EDO	D	212	4/4	0.91	0.15	41,43,43,44	0
9	MOH	A	240	2/2	0.91	0.17	39,39,39,39	0
8	EOH	A	235	3/3	0.91	0.20	31,31,38,42	0
8	EOH	D	231	3/3	0.92	0.16	44,44,51,64	0
8	EOH	C	231	3/3	0.92	0.21	61,61,63,63	0
9	MOH	D	240	2/2	0.93	0.13	54,54,54,57	0
8	EOH	D	236	3/3	0.93	0.58	50,50,55,61	0
8	EOH	D	226	3/3	0.93	0.22	46,46,50,50	0
8	EOH	D	225	3/3	0.94	0.12	33,33,35,42	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.



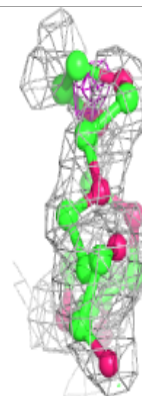
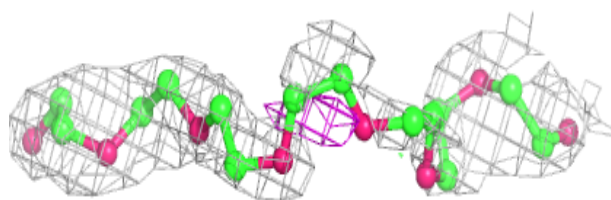
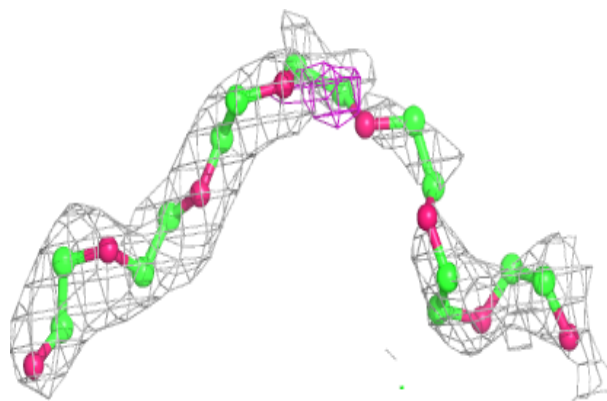
**Electron density around P6G D 209:**

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

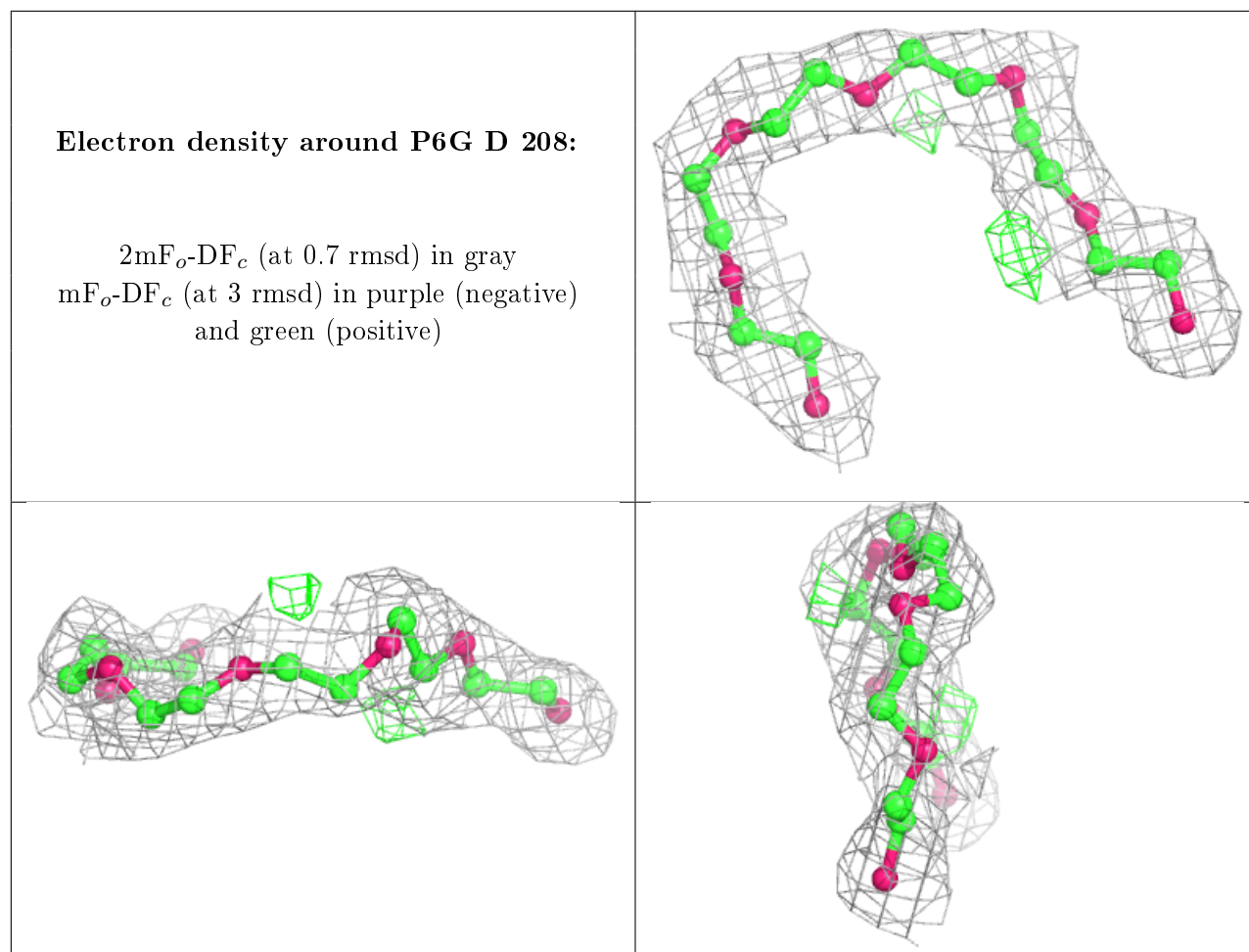


**Electron density around P33 C 207:**

$2mF_o-DF_c$  (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.