



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 21, 2026 – 02:23 PM EDT

PDB ID : 9PD9 / pdb\_00009pd9  
Title : The Structure of Porcine Trypsin in Complex with Crystallization Additives I  
Authors : McPherson, A.  
Deposited on : 2025-06-30  
Resolution : 1.28 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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 2.0  
EDS : 3.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

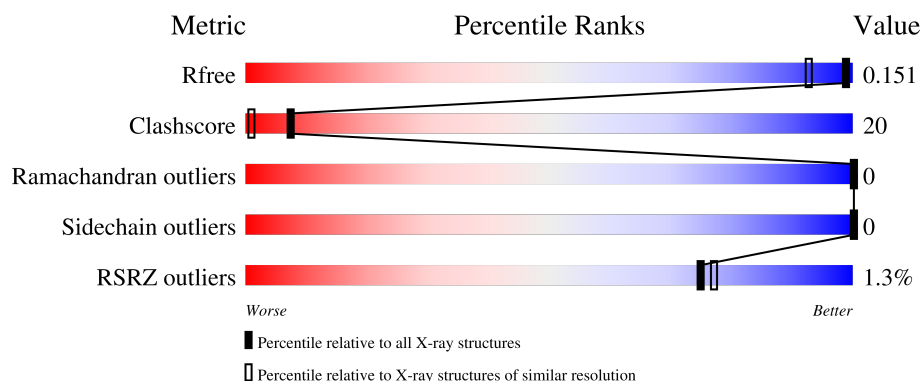
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.28 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))
$R_{free}$	180053	2836 (1.30-1.26)
Clashscore	190562	2911 (1.30-1.26)
Ramachandran outliers	187476	2841 (1.30-1.26)
Sidechain outliers	187428	2840 (1.30-1.26)
RSRZ outliers	180081	2832 (1.30-1.26)

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  $\geq 3$ , 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	231	<div> <div></div> <div>77%</div> <div>19%</div> <div>.</div> </div>

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	PG5	A	305	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	PEG	A	311	-	-	X	-
6	PG4	A	315	-	-	X	-
6	PG4	A	316	-	-	X	-
6	PG4	A	317	-	-	X	-
7	OXL	A	322	-	-	X	-
9	OXM	A	324[B]	-	X	-	-
9	OXM	A	326	-	X	-	-

## 2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 4779 atoms, of which 2338 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.

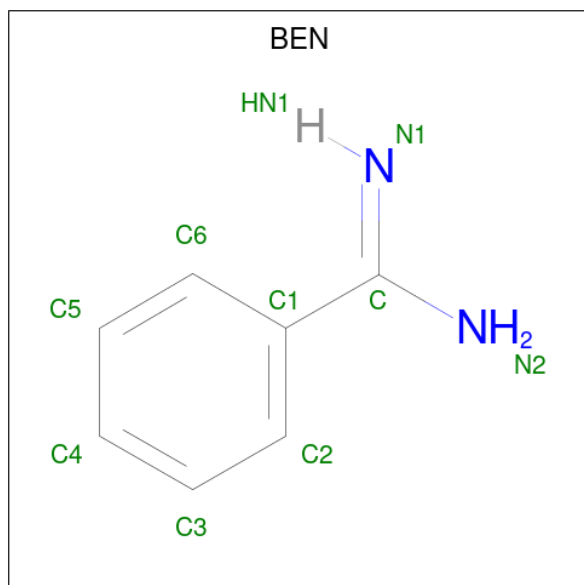
- Molecule 1 is a protein called Trypsin.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	223	Total	C	H	N	O	S	0	43	0
			3623	1109	1841	308	350	15			

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Ca	0	0
			1	1		

- Molecule 3 is BENZAMIDINE (CCD ID: BEN) (formula: C<sub>7</sub>H<sub>8</sub>N<sub>2</sub>).



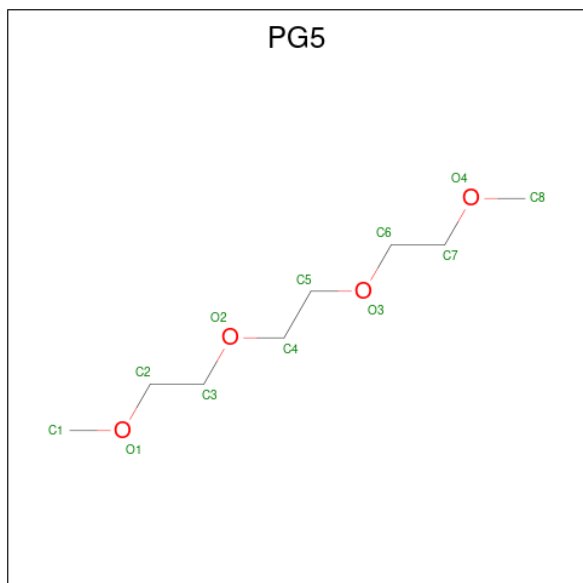
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	N	0	1
			32	14	14	4		
3	A	1	Total	C	H	N	0	0
			16	7	7	2		

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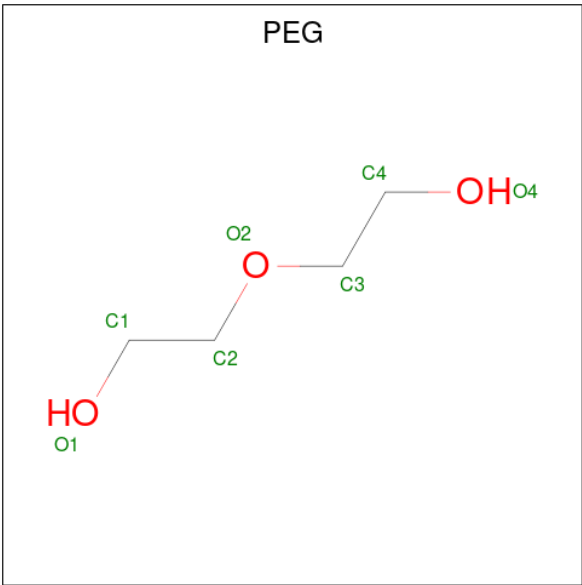
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	N	0	0
			17	7	8	2		
3	A	1	Total	C	H	N	0	0
			17	7	8	2		

- Molecule 4 is 1-METHOXY-2-[2-(2-METHOXY-ETHOXY)-ETHANE (CCD ID: PG5) (formula: C<sub>8</sub>H<sub>18</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	H	O	0	0
			30	8	18	4		
4	A	1	Total	C	H	O	0	0
			30	8	18	4		
4	A	1	Total	C	H	O	0	0
			30	8	18	4		
4	A	1	Total	C	H	O	0	0
			30	8	18	4		

- Molecule 5 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	H	O	0	0
			17	4	10	3		
5	A	1	Total	C	H	O	0	0
			17	4	10	3		
5	A	1	Total	C	H	O	0	0
			17	4	10	3		
5	A	1	Total	C	H	O	0	0
			15	4	9	2		
5	A	1	Total	C	H	O	0	0
			17	4	10	3		
5	A	1	Total	C	H	O	0	0
			17	4	10	3		
5	A	1	Total	C	H	O	0	0
			17	4	10	3		
5	A	1	Total	C	H	O	0	0
			17	4	10	3		
5	A	1	Total	C	H	O	0	0
			17	4	10	3		
5	A	1	Total	C	H	O	0	0
			17	4	10	3		
5	A	1	Total	C	H	O	0	0
			17	4	10	3		

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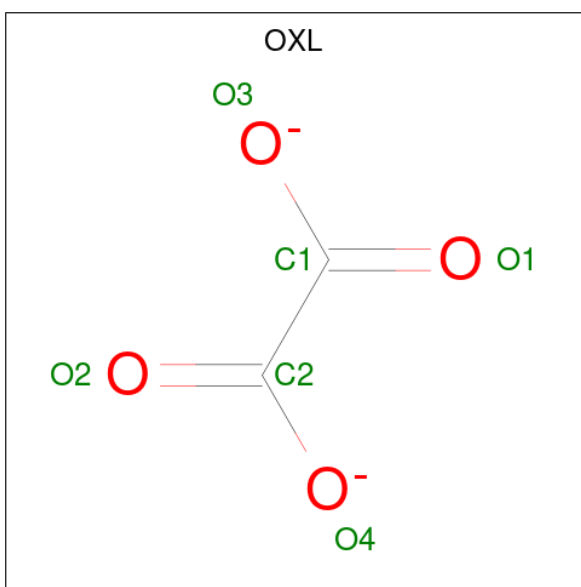
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	H	O	0	0
			17	4	10	3		

- Molecule 6 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula:  $C_8H_{18}O_5$ ).



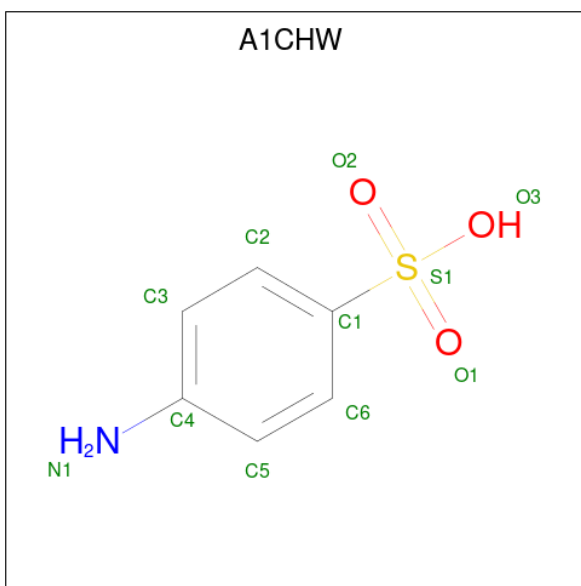
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	H	O	0	0
			31	8	18	5		
6	A	1	Total	C	H	O	0	0
			31	8	18	5		
6	A	1	Total	C	H	O	0	0
			31	8	18	5		
6	A	1	Total	C	H	O	0	0
			31	8	18	5		
6	A	1	Total	C	H	O	0	0
			31	8	18	5		
6	A	1	Total	C	H	O	0	0
			31	8	18	5		
6	A	1	Total	C	H	O	0	0
			31	8	18	5		

- Molecule 7 is OXALATE ION (CCD ID: OXL) (formula:  $C_2O_4$ ).



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

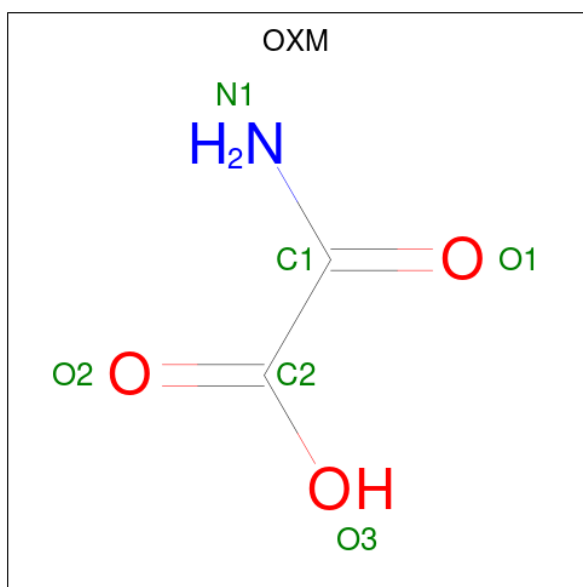
- Molecule 8 is 4-aminobenzene-1-sulfonic acid (CCD ID: A1CHW) (formula:  $C_6H_7NO_3S$ ).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
8	A	1	Total	C	H	N	O	S	0	0
			17	6	6	1	3	1		

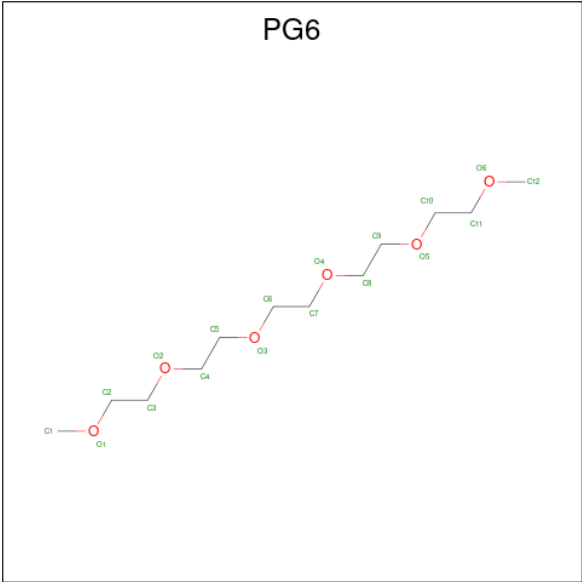
- Molecule 9 is OXAMIC ACID (CCD ID: OXM) (formula:  $C_2H_3NO_3$ ).





Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	A	1	Total	C	H	N	O	0	1
			8	2	2	1	3		
9	A	1	Total	C	H	N	O	0	1
			8	2	2	1	3		
9	A	1	Total	C	H	N	O	0	0
			8	2	2	1	3		
9	A	1	Total	C	H	N	O	0	0
			7	2	1	1	3		
9	A	1	Total	C	H	N	O	0	0
			8	2	2	1	3		
9	A	1	Total	C	H	N	O	0	0
			8	2	2	1	3		

- Molecule 10 is 1-(2-METHOXY-ETHOXY)-2-{2-[2-(2-METHOXY-ETHOXY)-ETHOXY]-ETHANE (CCD ID: PG6) (formula: C<sub>12</sub>H<sub>26</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	A	1	Total	C	H	O	0	0
			44	12	26	6		
10	A	1	Total	C	H	O	0	0
			44	12	26	6		
10	A	1	Total	C	H	O	0	0
			44	12	26	6		

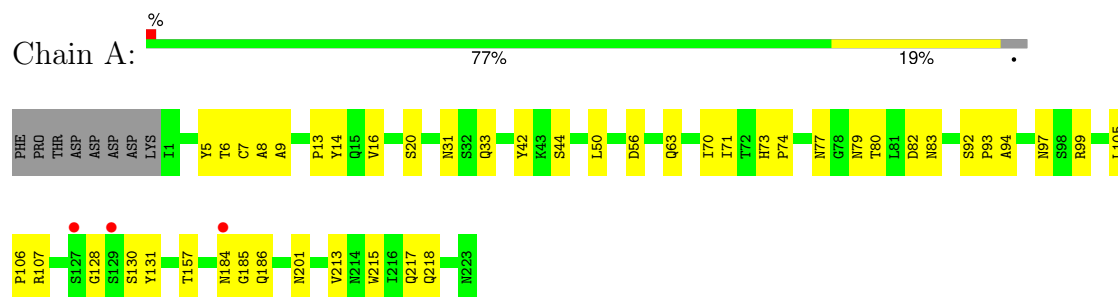
- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	236	Total	O	0	42
			250	250		

### 3 Residue-property plots

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

#### • Molecule 1: Trypsin



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	59.00Å 59.00Å 139.66Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.25 – 1.28 25.25 – 1.28	Depositor EDS
% Data completeness (in resolution range)	90.6 (25.25-1.28) 90.6 (25.25-1.28)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.02 (at 1.28Å)	Xtriage
Refinement program	PHENIX 1.21.1_5286	Depositor
R, $R_{free}$	0.113 , 0.147 0.124 , 0.151	Depositor DCC
$R_{free}$ test set	5907 reflections (9.18%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	17.4	Xtriage
Anisotropy	0.008	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 78.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.98	EDS
Total number of atoms	4779	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.35% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: A1CHW, OXL, PG6, PEG, PG4, PG5, CA, OXM, BEN

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	0.46	0/1998	0.62	0/2701

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1782	1841	1789	66	1
2	A	1	0	0	0	0
3	A	45	37	35	1	0
4	A	48	72	72	15	1
5	A	104	149	147	14	0
6	A	104	144	144	41	0
7	A	6	0	0	3	0
8	A	11	6	0	1	0
9	A	36	11	10	3	1
10	A	54	78	78	6	0
11	A	250	0	0	21	2
All	All	2441	2338	2275	92	3

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 20.

The worst 5 of 92 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:201[B]:ASN:OD1	11:A:401:HOH:O	1.70	1.05
1:A:6:THR:HB	6:A:315:PG4:H12	1.47	0.95
5:A:306:PEG:O4	11:A:402[A]:HOH:O	1.84	0.94
1:A:20[A]:SER:OG	11:A:403[A]:HOH:O	1.86	0.92
1:A:218[B]:GLN:OE1	11:A:404:HOH:O	1.88	0.90

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:325[B]:OXM:O3	11:A:445:HOH:O[7_645]	2.07	0.13
11:A:424:HOH:O	11:A:547:HOH:O[7_645]	2.16	0.04
1:A:79:ASN:HD22	4:A:305:PG5:O4[5_645]	1.58	0.02

## 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	263/231 (114%)	258 (98%)	5 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	225/191 (118%)	225 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	217	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

Of 44 ligands modelled in this entry, 1 is 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	$\# Z  > 2$
5	PEG	A	313	-	6,6,6	0.26	0	5,5,5	0.31	0
6	PG4	A	317	-	12,12,12	0.32	0	11,11,11	0.25	0
3	BEN	A	302[B]	-	9,9,9	0.54	0	7,11,11	0.48	0
9	OXM	A	327	-	5,5,5	1.28	1 (20%)	2,6,6	1.34	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
9	OXM	A	328	-	5,5,5	1.30	1 (20%)	2,6,6	1.05	0
5	PEG	A	337	-	6,6,6	0.28	0	5,5,5	0.21	0
5	PEG	A	341	-	6,6,6	0.25	0	5,5,5	0.26	0
7	OXL	A	322	-	5,5,5	1.64	0	6,6,6	1.46	1 (16%)
5	PEG	A	343	-	6,6,6	0.23	0	5,5,5	0.18	0
4	PG5	A	305	-	11,11,11	0.38	0	10,10,10	0.48	0
5	PEG	A	340	-	6,6,6	0.24	0	5,5,5	0.29	0
6	PG4	A	316	-	12,12,12	0.30	0	11,11,11	0.51	0
5	PEG	A	338	-	6,6,6	0.25	0	5,5,5	0.33	0
5	PEG	A	335	-	6,6,6	0.25	0	5,5,5	0.25	0
4	PG5	A	304	-	11,11,11	0.51	0	10,10,10	0.55	0
10	PG6	A	331	-	17,17,17	0.34	0	16,16,16	0.22	0
8	A1CHW	A	323	-	11,11,11	0.53	0	16,16,16	1.07	1 (6%)
4	PG5	A	310	-	11,11,11	0.36	0	10,10,10	0.39	0
3	BEN	A	303	-	9,9,9	0.49	0	7,11,11	1.37	1 (14%)
5	PEG	A	309	-	6,6,6	0.26	0	5,5,5	0.20	0
9	OXM	A	324[B]	-	5,5,5	2.16	3 (60%)	2,6,6	3.61	2 (100%)
5	PEG	A	311	-	6,6,6	0.30	0	5,5,5	0.70	0
5	PEG	A	342	-	6,6,6	0.24	0	5,5,5	0.44	0
6	PG4	A	321	-	12,12,12	0.40	0	11,11,11	0.54	0
3	BEN	A	330	-	9,9,9	0.61	0	7,11,11	0.74	0
9	OXM	A	326	-	5,5,5	1.19	1 (20%)	2,6,6	1.44	1 (50%)
3	BEN	A	336	-	9,9,9	0.61	0	7,11,11	0.78	0
4	PG5	A	334	-	11,11,11	0.36	0	10,10,10	0.25	0
5	PEG	A	314	-	6,6,6	0.29	0	5,5,5	0.23	0
5	PEG	A	308	-	6,6,6	0.25	0	5,5,5	0.30	0
6	PG4	A	315	-	12,12,12	0.35	0	11,11,11	0.39	0
9	OXM	A	325[B]	-	5,5,5	1.15	1 (20%)	2,6,6	1.87	1 (50%)
10	PG6	A	332	-	17,17,17	0.35	0	16,16,16	0.46	0
5	PEG	A	339	-	6,6,6	0.28	0	5,5,5	0.58	0
6	PG4	A	320	-	12,12,12	0.32	0	11,11,11	0.54	0
9	OXM	A	329	-	5,5,5	1.14	0	2,6,6	1.46	1 (50%)
6	PG4	A	307	-	12,12,12	0.33	0	11,11,11	0.32	0
10	PG6	A	333	-	17,17,17	0.35	0	16,16,16	0.13	0
5	PEG	A	312	-	5,5,6	0.31	0	4,4,5	0.26	0
5	PEG	A	306	-	6,6,6	0.32	0	5,5,5	0.41	0
3	BEN	A	302[A]	-	9,9,9	0.60	0	7,11,11	0.57	0
6	PG4	A	319	-	12,12,12	0.31	0	11,11,11	0.28	0
6	PG4	A	318	-	12,12,12	0.33	0	11,11,11	0.45	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	PEG	A	313	-	-	1/4/4/4	-
6	PG4	A	317	-	-	6/10/10/10	-
3	BEN	A	302[B]	-	-	0/4/4/4	0/1/1/1
9	OXM	A	327	-	-	0/4/4/4	-
9	OXM	A	328	-	-	0/4/4/4	-
5	PEG	A	337	-	-	1/4/4/4	-
5	PEG	A	341	-	-	3/4/4/4	-
7	OXL	A	322	-	-	4/4/4/4	-
5	PEG	A	343	-	-	2/4/4/4	-
4	PG5	A	305	-	-	3/9/9/9	-
5	PEG	A	340	-	-	3/4/4/4	-
6	PG4	A	316	-	-	8/10/10/10	-
5	PEG	A	338	-	-	4/4/4/4	-
5	PEG	A	335	-	-	2/4/4/4	-
4	PG5	A	304	-	-	5/9/9/9	-
10	PG6	A	331	-	-	8/15/15/15	-
8	A1CHW	A	323	-	-	0/6/6/6	0/1/1/1
4	PG5	A	310	-	-	4/9/9/9	-
3	BEN	A	303	-	-	2/4/4/4	0/1/1/1
5	PEG	A	309	-	-	3/4/4/4	-
9	OXM	A	324[B]	-	-	4/4/4/4	-
5	PEG	A	311	-	-	2/4/4/4	-
5	PEG	A	342	-	-	2/4/4/4	-
6	PG4	A	321	-	-	6/10/10/10	-
3	BEN	A	330	-	-	0/4/4/4	0/1/1/1
9	OXM	A	326	-	-	4/4/4/4	-
3	BEN	A	336	-	-	4/4/4/4	0/1/1/1
4	PG5	A	334	-	-	6/9/9/9	-
5	PEG	A	314	-	-	3/4/4/4	-
5	PEG	A	308	-	-	1/4/4/4	-
6	PG4	A	315	-	-	4/10/10/10	-
9	OXM	A	325[B]	-	-	0/4/4/4	-
10	PG6	A	332	-	-	10/15/15/15	-
5	PEG	A	339	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	PG4	A	320	-	-	4/10/10/10	-
9	OXM	A	329	-	-	4/4/4/4	-
6	PG4	A	307	-	-	5/10/10/10	-
10	PG6	A	333	-	-	7/15/15/15	-
5	PEG	A	312	-	-	1/3/3/4	-
5	PEG	A	306	-	-	2/4/4/4	-
3	BEN	A	302[A]	-	-	4/4/4/4	0/1/1/1
6	PG4	A	319	-	-	5/10/10/10	-
6	PG4	A	318	-	-	9/10/10/10	-

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	324[B]	OXM	C1-C2	-3.41	1.51	1.55
9	A	324[B]	OXM	O3-C2	-2.65	1.23	1.30
9	A	325[B]	OXM	O3-C2	-2.23	1.24	1.30
9	A	328	OXM	O3-C2	-2.17	1.24	1.30
9	A	326	OXM	O3-C2	-2.15	1.24	1.30

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	324[B]	OXM	O3-C2-O2	4.35	134.25	123.90
9	A	324[B]	OXM	O1-C1-N1	2.68	128.91	122.89
9	A	325[B]	OXM	O3-C2-O2	2.45	129.74	123.90
8	A	323	A1CHW	C5-C6-C1	2.14	121.52	119.44
7	A	322	OXL	O3-C1-C2	2.10	116.91	112.83

There are no chirality outliers.

5 of 148 torsion outliers are listed below:

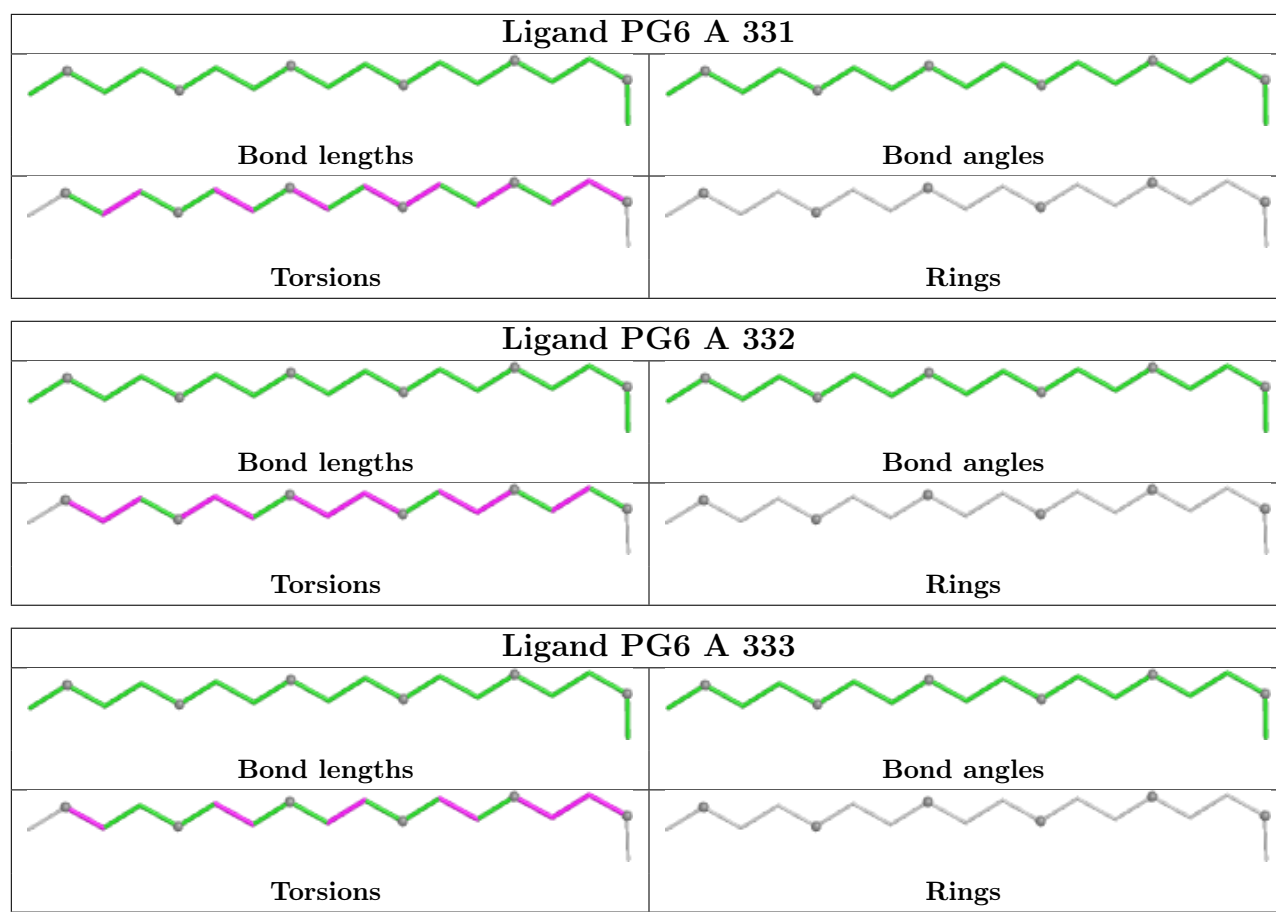
Mol	Chain	Res	Type	Atoms
3	A	336	BEN	N2-C-C1-C2
3	A	336	BEN	N1-C-C1-C6
3	A	336	BEN	N2-C-C1-C6
7	A	322	OXL	O1-C1-C2-O2
7	A	322	OXL	O1-C1-C2-O4

There are no ring outliers.

25 monomers are involved in 82 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	313	PEG	1	0
6	A	317	PG4	7	0
9	A	327	OXM	1	0
9	A	328	OXM	1	0
5	A	341	PEG	1	0
7	A	322	OXL	3	0
4	A	305	PG5	10	1
6	A	316	PG4	7	0
4	A	304	PG5	4	0
8	A	323	A1CHW	1	0
4	A	310	PG5	3	0
5	A	311	PEG	6	0
6	A	321	PG4	3	0
6	A	315	PG4	8	0
9	A	325[B]	OXM	0	1
10	A	332	PG6	6	0
5	A	339	PEG	2	0
6	A	320	PG4	6	0
9	A	329	OXM	1	0
6	A	307	PG4	3	0
5	A	312	PEG	1	0
5	A	306	PEG	3	0
3	A	302[A]	BEN	1	0
6	A	319	PG4	4	0
6	A	318	PG4	6	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	223/231 (96%)	-0.72	3 (1%) 75 77	10, 20, 33, 52	44 (19%)

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	184[A]	ASN	2.7
1	A	127[A]	SER	2.3
1	A	129[A]	SER	2.1

### 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 oligosaccharides 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(Å <sup>2</sup> )	Q<0.9
5	PEG	A	337	7/7	0.31	0.16	54,77,91,100	17
10	PG6	A	333	18/18	0.32	0.15	39,78,95,100	44
4	PG5	A	334	12/12	0.36	0.13	44,80,103,104	30
5	PEG	A	342	7/7	0.40	0.18	40,60,82,89	17

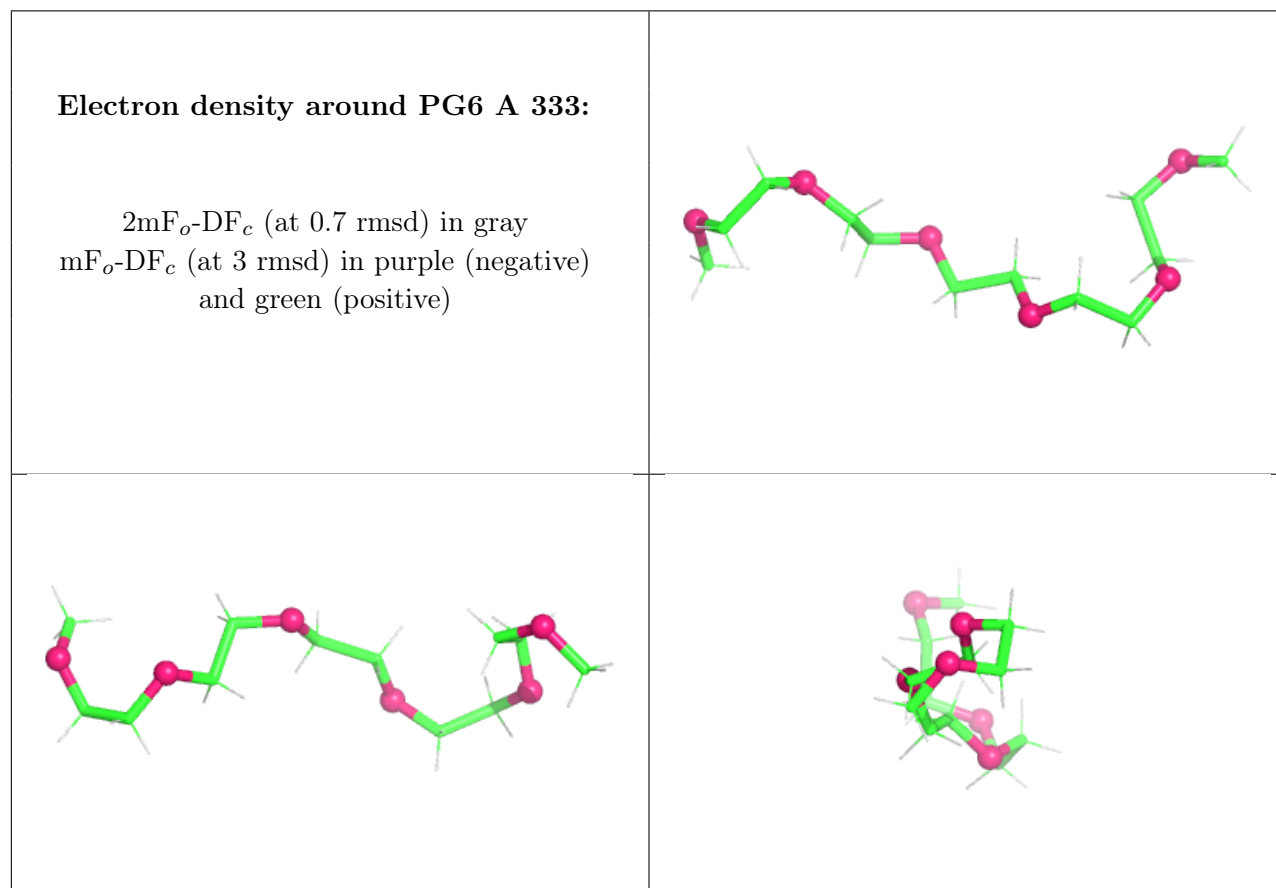
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	BEN	A	336	9/9	0.41	0.16	61,77,104,125	17
5	PEG	A	308	7/7	0.47	0.12	45,64,94,94	17
5	PEG	A	341	7/7	0.47	0.15	49,64,91,91	17
5	PEG	A	335	7/7	0.48	0.11	61,81,97,97	17
5	PEG	A	343	7/7	0.56	0.13	51,64,79,90	17
9	OXM	A	328	6/6	0.57	0.15	117,167,181,183	0
5	PEG	A	314	7/7	0.60	0.20	35,54,97,115	17
5	PEG	A	309	7/7	0.60	0.11	57,70,97,97	17
5	PEG	A	338	7/7	0.61	0.12	51,75,92,92	17
3	BEN	A	330	9/9	0.61	0.18	102,138,167,186	0
5	PEG	A	313	7/7	0.65	0.14	48,65,79,79	17
5	PEG	A	339	7/7	0.66	0.15	52,72,87,97	17
3	BEN	A	302[A]	9/9	0.66	0.20	80,83,99,100	16
3	BEN	A	302[B]	9/9	0.66	0.20	75,78,94,94	16
10	PG6	A	331	18/18	0.68	0.22	93,114,123,123	44
6	PG4	A	319	13/13	0.68	0.23	74,176,211,235	0
7	OXL	A	322	6/6	0.69	0.13	52,64,75,81	6
6	PG4	A	316	13/13	0.69	0.20	29,60,90,96	31
4	PG5	A	305	12/12	0.70	0.23	45,59,80,89	30
5	PEG	A	340	7/7	0.71	0.15	42,67,89,89	17
9	OXM	A	329	6/6	0.74	0.21	92,146,190,198	0
6	PG4	A	318	13/13	0.75	0.21	26,52,69,77	31
5	PEG	A	312	6/7	0.76	0.19	33,57,89,89	15
9	OXM	A	327	6/6	0.76	0.16	106,170,183,204	0
10	PG6	A	332	18/18	0.77	0.26	26,46,75,90	44
4	PG5	A	304	12/12	0.77	0.25	39,81,104,109	30
5	PEG	A	306	7/7	0.78	0.20	28,40,85,90	17
6	PG4	A	317	13/13	0.79	0.18	27,58,91,109	31
6	PG4	A	320	13/13	0.80	0.21	26,73,99,105	31
6	PG4	A	307	13/13	0.80	0.20	28,58,100,110	31
6	PG4	A	315	13/13	0.81	0.21	29,55,102,117	31
4	PG5	A	310	12/12	0.82	0.17	31,59,81,97	30
9	OXM	A	326	6/6	0.84	0.17	60,124,167,193	0
9	OXM	A	324[B]	6/6	0.85	0.16	30,35,42,42	8
6	PG4	A	321	13/13	0.85	0.18	22,56,104,113	31
5	PEG	A	311	7/7	0.86	0.16	31,61,86,86	17
9	OXM	A	325[B]	6/6	0.88	0.13	51,51,63,63	8
8	A1CHW	A	323	11/11	0.99	0.03	20,22,33,33	0
3	BEN	A	303	9/9	0.99	0.04	16,19,25,27	0
2	CA	A	301	1/1	1.00	0.02	17,17,17,17	1

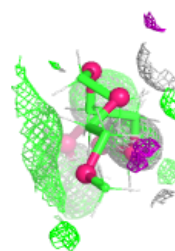
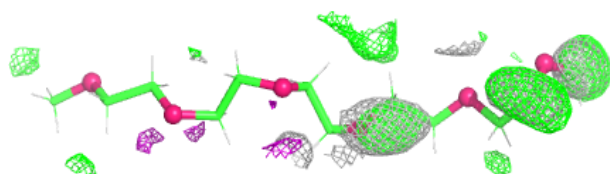
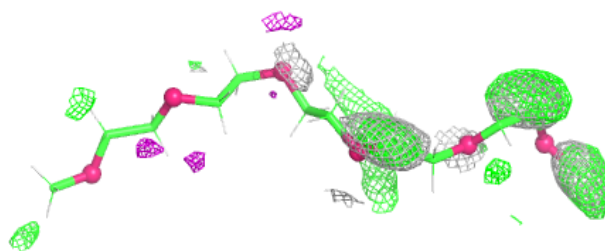
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers

as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

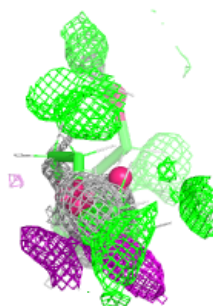
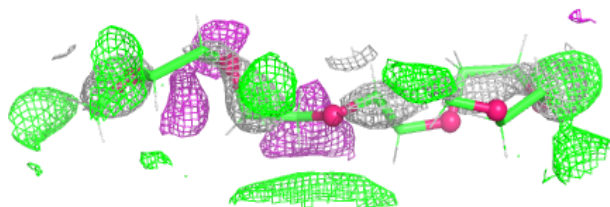
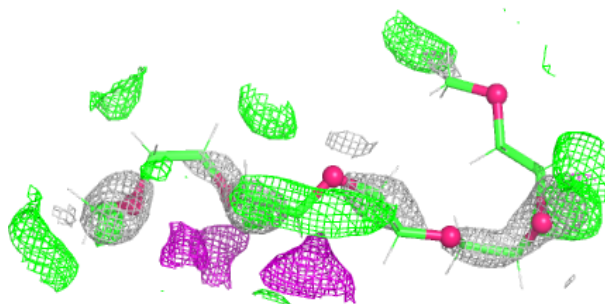


**Electron density around PG6 A 331:**

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

**Electron density around PG6 A 332:**

$2mF_o-DF_c$  (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.