



# wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 16, 2025 – 04:16 AM EDT

PDB ID : 9PDA / pdb\_00009pda  
Title : Structure of Porcine Trypsin Crystals Grown From PEG and Complexed With Crystallization Additives IV  
Authors : McPherson, A.  
Deposited on : 2025-06-30  
Resolution : 1.18 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 Phenix2.0rc1  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 2.0rc1  
EDS : 3.0  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.006 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.45.1

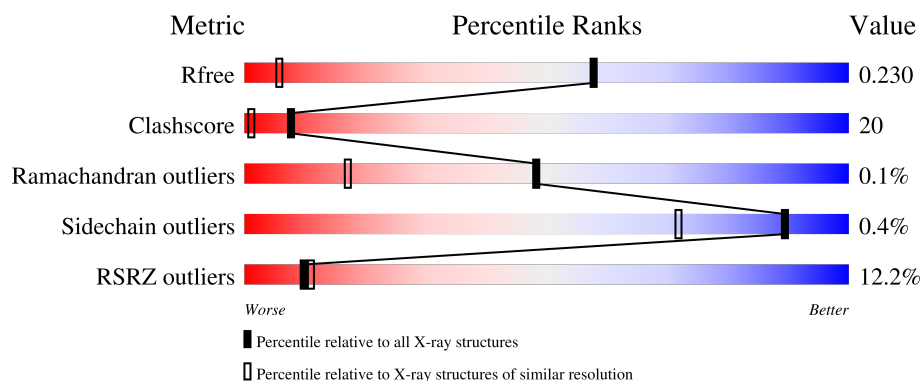
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.18 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))
$R_{free}$	164625	1569 (1.20-1.16)
Clashscore	180529	1711 (1.20-1.16)
Ramachandran outliers	177936	1657 (1.20-1.16)
Sidechain outliers	177891	1657 (1.20-1.16)
RSRZ outliers	164620	1568 (1.20-1.16)

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	
1	B	231	
1	C	231	
1	D	231	

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
2	BEN	C	301	-	-	X	-
5	PEG	B	325	-	-	X	-
5	PEG	C	308	-	-	X	-
5	PEG	C	309	-	-	X	-
5	PEG	C	312	-	-	X	-
5	PEG	C	316	-	-	X	-
5	PEG	D	319	-	-	X	-
5	PEG	D	320	-	-	X	-
5	PEG	D	321	-	-	X	-
8	PG4	D	333	-	-	X	-

## 2 Entry composition [i](#)

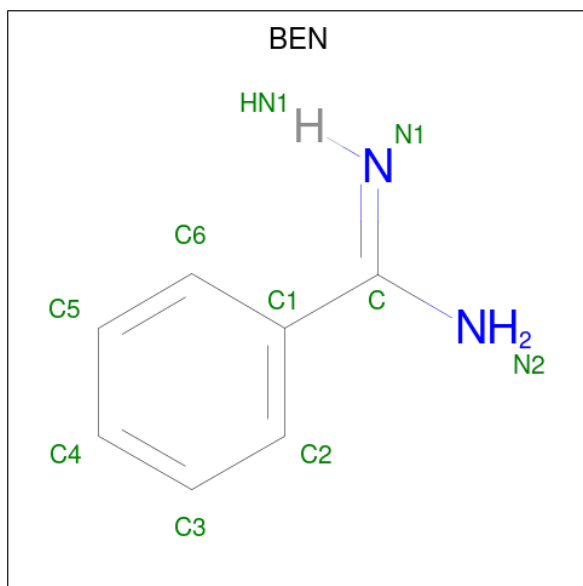
There are 12 unique types of molecules in this entry. The entry contains 16671 atoms, of which 7751 are hydrogens and 0 are deuteriums.

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	2	0
			3258	1027	1604	288	325	14			
1	B	223	Total	C	H	N	O	S	0	1	0
			3238	1020	1596	287	321	14			
1	C	223	Total	C	H	N	O	S	0	0	0
			3237	1020	1595	287	321	14			
1	D	223	Total	C	H	N	O	S	0	5	0
			3293	1038	1624	291	326	14			

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



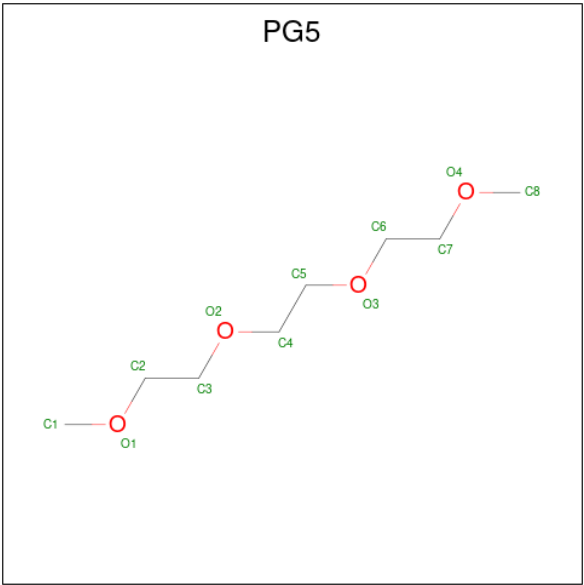
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	H	N	0	0
			17	7	8	2		
2	B	1	Total	C	H	N	0	0
			17	7	8	2		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	H	N	0	0
			17	7	8	2		
2	B	1	Total	C	H	N	0	0
			17	7	8	2		
2	C	1	Total	C	H	N	0	0
			17	7	8	2		
2	C	1	Total	C	H	N	0	0
			17	7	8	2		
2	C	1	Total	C	H	N	0	0
			17	7	8	2		
2	D	1	Total	C	H	N	0	0
			17	7	8	2		
2	D	1	Total	C	H	N	0	1
			34	14	16	4		
2	D	1	Total	C	H	N	0	0
			17	7	8	2		

- Molecule 3 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>).



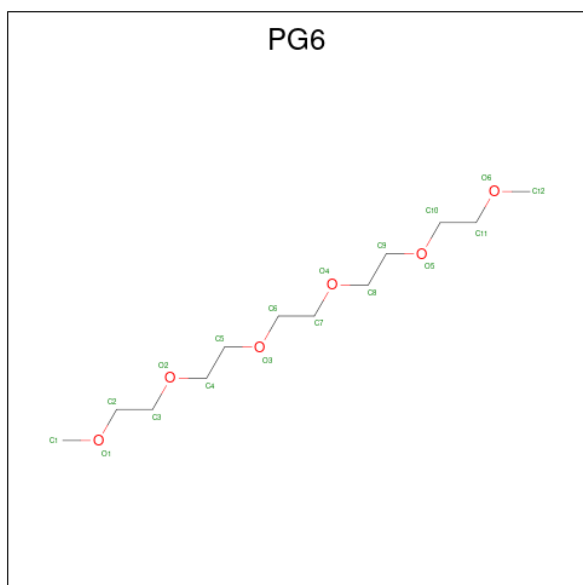
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O	0	0
			30	8	18	4		
3	A	1	Total	C	H	O	0	0
			30	8	18	4		
3	A	1	Total	C	H	O	0	0
			30	8	18	4		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	H	O	0	0
			30	8	18	4		
3	B	1	Total	C	H	O	0	0
			30	8	18	4		
3	B	1	Total	C	H	O	0	0
			30	8	18	4		
3	B	1	Total	C	H	O	0	0
			30	8	18	4		
3	C	1	Total	C	H	O	0	0
			30	8	18	4		
3	C	1	Total	C	H	O	0	0
			30	8	18	4		
3	D	1	Total	C	H	O	0	0
			29	8	17	4		
3	D	1	Total	C	H	O	0	0
			30	8	18	4		
3	D	1	Total	C	H	O	0	0
			30	8	18	4		

- Molecule 4 is 1-(2-METHOXY-ETHOXY)-2-{2-[2-(2-METHOXY-ETHOXY)-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
4	A	1	Total	C	H	O	0	0
			44	12	26	6		

- 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
			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	B	1	Total	C	H	O	0	0
			17	4	10	3		
5	B	1	Total	C	H	O	0	0
			17	4	10	3		
5	B	1	Total	C	H	O	0	0
			17	4	10	3		
5	B	1	Total	C	H	O	0	0
			17	4	10	3		
5	B	1	Total	C	H	O	0	0
			17	4	10	3		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	C	H	O	0	0
			17	4	10	3		
5	B	1	Total	C	H	O	0	0
			17	4	10	3		
5	B	1	Total	C	H	O	0	0
			17	4	10	3		
5	B	1	Total	C	H	O	0	1
			34	8	20	6		
5	B	1	Total	C	H	O	0	0
			17	4	10	3		
5	B	1	Total	C	H	O	0	0
			17	4	10	3		
5	B	1	Total	C	H	O	0	0
			17	4	10	3		
5	B	1	Total	C	H	O	0	0
			17	4	10	3		
5	B	1	Total	C	H	O	0	0
			17	4	10	3		
5	B	1	Total	C	H	O	0	0
			16	4	9	3		
5	B	1	Total	C	H	O	0	0
			17	4	10	3		
5	C	1	Total	C	H	O	0	0
			17	4	10	3		
5	C	1	Total	C	H	O	0	0
			17	4	10	3		
5	C	1	Total	C	H	O	0	0
			17	4	10	3		
5	C	1	Total	C	H	O	0	0
			17	4	10	3		
5	C	1	Total	C	H	O	0	0
			17	4	10	3		
5	C	1	Total	C	H	O	0	0
			17	4	10	3		
5	C	1	Total	C	H	O	0	0
			17	4	10	3		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	C	1	Total	C	H	O	0	0
			17	4	10	3		
5	C	1	Total	C	H	O	0	0
			17	4	10	3		
5	C	1	Total	C	H	O	0	0
			17	4	10	3		
5	C	1	Total	C	H	O	0	0
			17	4	10	3		
5	C	1	Total	C	H	O	0	0
			17	4	10	3		
5	C	1	Total	C	H	O	0	1
			34	8	20	6		
5	D	1	Total	C	H	O	0	0
			17	4	10	3		
5	D	1	Total	C	H	O	0	0
			17	4	10	3		
5	D	1	Total	C	H	O	0	0
			17	4	10	3		
5	D	1	Total	C	H	O	0	0
			17	4	10	3		
5	D	1	Total	C	H	O	0	0
			17	4	10	3		
5	D	1	Total	C	H	O	0	1
			34	8	20	6		
5	D	1	Total	C	H	O	0	0
			16	4	9	3		
5	D	1	Total	C	H	O	0	0
			15	4	8	3		
5	D	1	Total	C	H	O	0	0
			17	4	10	3		
5	D	1	Total	C	H	O	0	0
			17	4	10	3		
5	D	1	Total	C	H	O	0	0
			17	4	10	3		
5	D	1	Total	C	H	O	0	0
			17	4	10	3		
5	D	1	Total	C	H	O	0	0
			17	4	10	3		
5	D	1	Total	C	H	O	0	0
			17	4	10	3		

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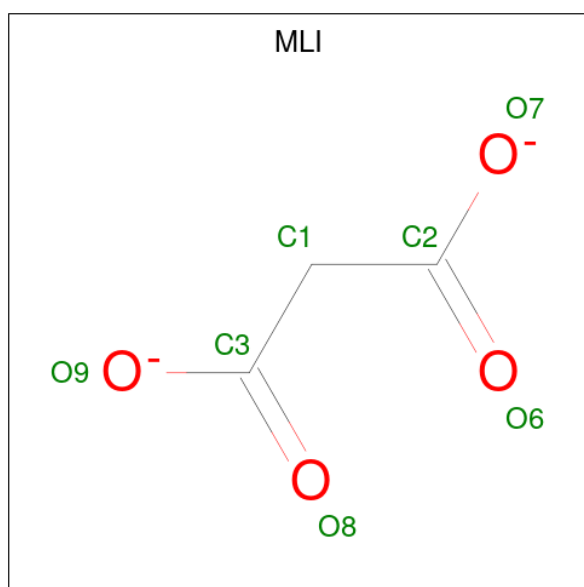
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	D	1	Total	C	H	O	0	0
			17	4	10	3		
5	D	1	Total	C	H	O	0	0
			17	4	10	3		
5	D	1	Total	C	H	O	0	0
			17	4	10	3		
5	D	1	Total	C	H	O	0	0
			17	4	10	3		
5	D	1	Total	C	H	O	0	0
			17	4	10	3		

- Molecule 6 is CALCIUM ION (CCD ID: CA) (formula: Ca).

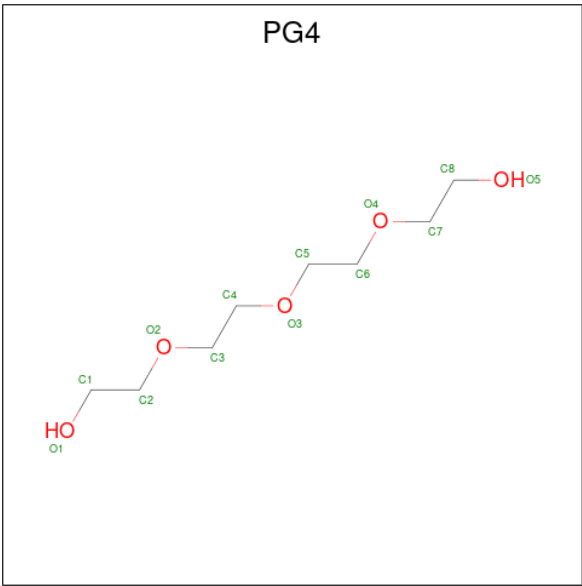
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Ca	0	0
			1	1		
6	B	1	Total	Ca	0	0
			1	1		
6	C	1	Total	Ca	0	0
			1	1		
6	D	2	Total	Ca	0	0
			2	2		

- Molecule 7 is MALONATE ION (CCD ID: MLI) (formula: C<sub>3</sub>H<sub>2</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	H	O	0	0
			9	3	2	4		
7	B	1	Total	C	H	O	0	0
			9	3	2	4		
7	C	1	Total	C	H	O	0	0
			9	3	2	4		
7	D	1	Total	C	H	O	0	0
			9	3	2	4		

- Molecule 8 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: C<sub>8</sub>H<sub>18</sub>O<sub>5</sub>).



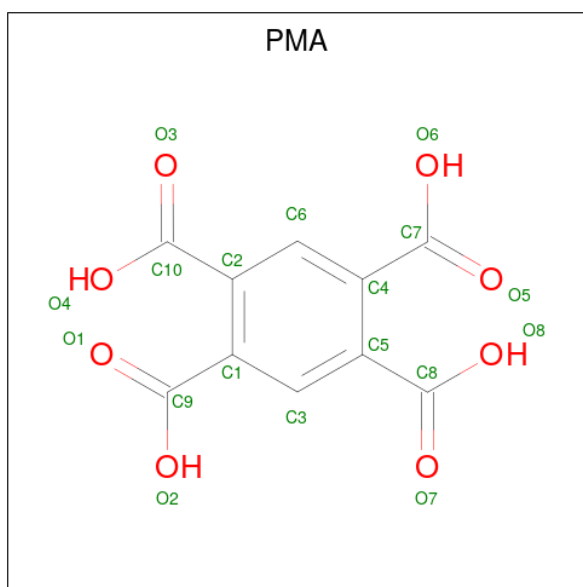
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total	C	H	O	0	0
			29	8	17	4		
8	A	1	Total	C	H	O	0	0
			30	8	17	5		
8	A	1	Total	C	H	O	0	0
			31	8	18	5		
8	A	1	Total	C	H	O	0	0
			31	8	18	5		
8	B	1	Total	C	H	O	0	0
			31	8	18	5		
8	B	1	Total	C	H	O	0	0
			31	8	18	5		
8	B	1	Total	C	H	O	0	0
			31	8	18	5		
8	C	1	Total	C	H	O	0	0
			31	8	18	5		

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

- Molecule 9 is PYROMELLITIC ACID (CCD ID: PMA) (formula:  $C_{10}H_6O_8$ ) (labeled as "Ligand of Interest" by depositor).



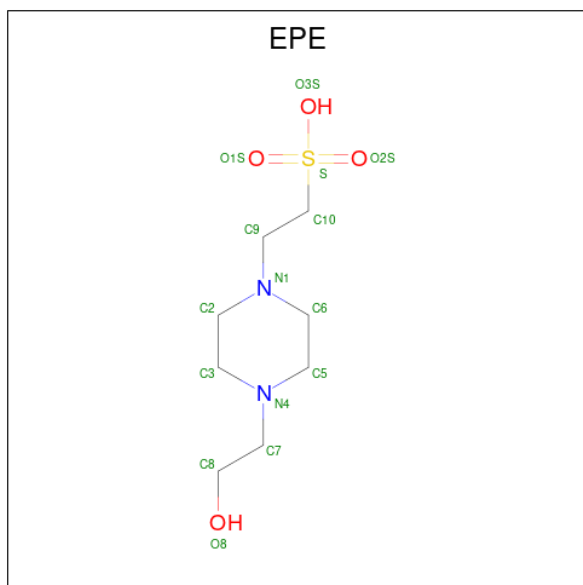
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	B	1	Total	C	H	O	0	0
			20	10	2	8		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	D	1	Total	C	H	O	0	0
			20	10	2	8		

- Molecule 10 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (CCD ID: EPE) (formula: C<sub>8</sub>H<sub>18</sub>N<sub>2</sub>O<sub>4</sub>S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
10	C	1	Total	C	H	N	O	S	0	0
			31	8	16	2	4	1		
10	D	1	Total	C	H	N	O	S	0	0
			32	8	17	2	4	1		

- Molecule 11 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	D	1	Total	Cl	0	0
			1	1		

- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	292	Total	O	0	7
			294	294		
12	B	263	Total	O	0	14
			269	269		

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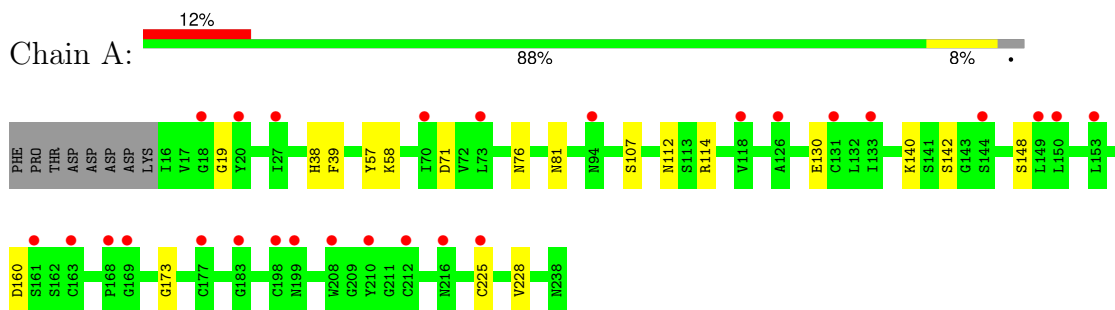
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	C	358	Total 361	O 361	0	8
12	D	344	Total 347	O 347	0	6

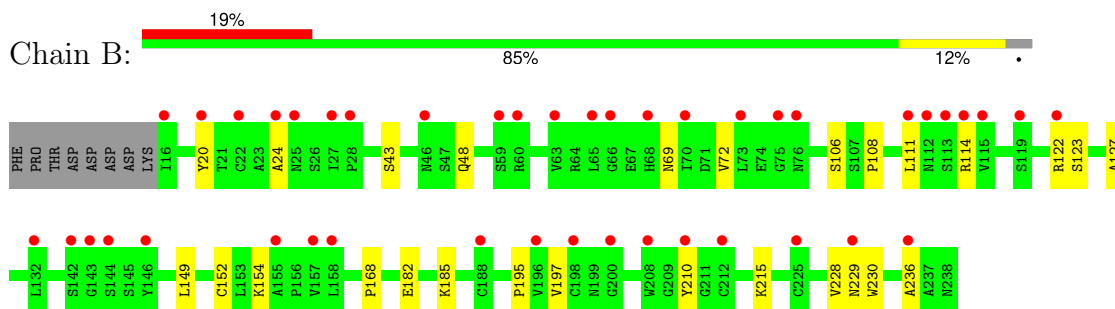
### 3 Residue-property plots [i](#)

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.

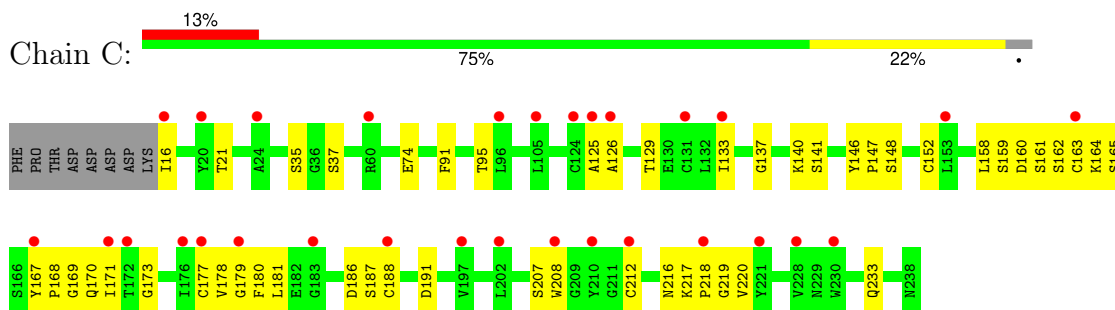
#### • Molecule 1: Trypsin



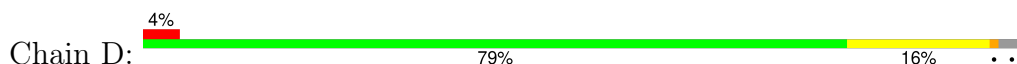
#### • Molecule 1: Trypsin

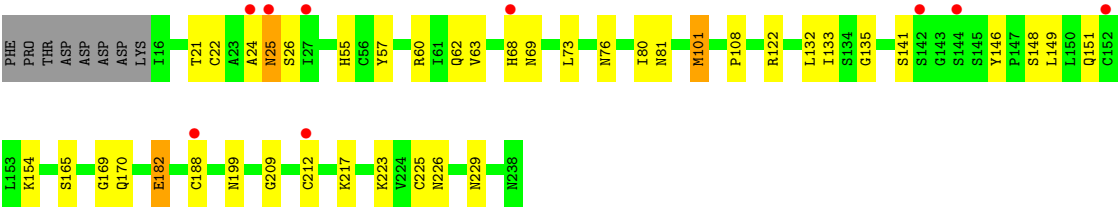


#### • Molecule 1: Trypsin



#### • Molecule 1: Trypsin







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	70.66Å 50.72Å 125.69Å 90.00° 99.52° 90.00°	Depositor
Resolution (Å)	39.25 – 1.18 39.25 – 1.18	Depositor EDS
% Data completeness (in resolution range)	91.1 (39.25-1.18) 91.1 (39.25-1.18)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.60 (at 1.18Å)	Xtriage
Refinement program	PHENIX 1.21.1_5286	Depositor
R, $R_{free}$	0.195 , 0.230 0.195 , 0.230	Depositor DCC
$R_{free}$ test set	13014 reflections (4.52%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	15.5	Xtriage
Anisotropy	0.214	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 45.3	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	0.97	EDS
Total number of atoms	16671	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 76.22 % 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 1.0847e-06. 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: PG6, MLI, PG4, CA, PG5, PMA, PEG, CL, EPE, 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	0.55	0/1689	0.71	0/2293
1	B	0.47	0/1674	0.63	0/2273
1	C	0.61	0/1674	0.74	0/2273
1	D	0.62	0/1713	0.74	1/2326 (0.0%)
All	All	0.56	0/6750	0.71	1/9165 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	101	MET	CA-CB-CG	5.32	124.73	114.10

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	1654	1604	1605	18	3
1	B	1642	1596	1595	31	1
1	C	1642	1595	1595	105	0
1	D	1669	1624	1630	69	2
2	A	9	8	7	0	0
2	B	27	24	21	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	27	24	21	4	0
2	D	36	32	28	1	0
3	A	36	54	54	6	0
3	B	48	72	72	8	0
3	C	24	36	36	4	0
3	D	36	53	54	8	0
4	A	18	26	26	2	0
5	A	56	80	80	3	0
5	B	133	189	190	24	0
5	C	112	160	160	26	0
5	D	147	207	210	27	1
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	2	0	0	0	0
7	A	7	2	2	1	0
7	B	7	2	2	1	0
7	C	7	2	2	0	0
7	D	7	2	2	0	0
8	A	51	70	69	3	2
8	B	39	54	54	7	0
8	C	65	90	90	11	0
8	D	78	108	108	14	4
9	B	18	2	2	3	0
9	D	18	2	2	4	0
10	C	15	16	18	3	0
10	D	15	17	17	3	0
11	D	1	0	0	0	1
12	A	294	0	0	13	10
12	B	269	0	0	23	10
12	C	361	0	0	97	14
12	D	347	0	0	61	5
All	All	8920	7751	7752	303	28

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 303 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:225:CYS:SG	12:D:419:HOH:O	1.92	1.26

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:177:CYS:SG	12:C:679:HOH:O	1.91	1.25
1:D:101:MET:SD	12:D:682:HOH:O	1.96	1.22
1:C:188:CYS:SG	12:C:580:HOH:O	2.02	1.18
1:C:163:CYS:SG	12:C:679:HOH:O	2.02	1.15

The worst 5 of 28 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)
12:B:602:HOH:O	12:C:683:HOH:O[1_545]	1.38	0.82
11:D:338:CL:CL	12:A:609:HOH:O[1_554]	1.58	0.62
8:D:333:PG4:O1	12:C:725:HOH:O[2_745]	1.68	0.52
12:A:404:HOH:O	12:C:651:HOH:O[2_746]	1.75	0.45
12:C:641:HOH:O	12:D:426:HOH:O[2_755]	1.75	0.45

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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	223/231 (96%)	217 (97%)	6 (3%)	0	100	100
1	B	221/231 (96%)	217 (98%)	4 (2%)	0	100	100
1	C	221/231 (96%)	217 (98%)	4 (2%)	0	100	100
1	D	226/231 (98%)	218 (96%)	6 (3%)	2 (1%)	14	1
All	All	891/924 (96%)	869 (98%)	20 (2%)	2 (0%)	48	16

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	25[A]	ASN
1	D	25[B]	ASN

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	185/191 (97%)	185 (100%)	0	100	100
1	B	183/191 (96%)	181 (99%)	2 (1%)	70	36
1	C	183/191 (96%)	183 (100%)	0	100	100
1	D	188/191 (98%)	187 (100%)	1 (0%)	86	64
All	All	739/764 (97%)	736 (100%)	3 (0%)	89	72

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	182	GLU
1	B	185	LYS
1	D	182	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	151	GLN
1	C	233	GLN
1	D	203	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 [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 120 ligands modelled in this entry, 6 are monoatomic - leaving 114 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	D	308	-	6,6,6	0.21	0	5,5,5	0.43	0
5	PEG	D	334	-	6,6,6	0.24	0	5,5,5	0.23	0
3	PG5	B	307	-	11,11,11	0.31	0	10,10,10	0.20	0
8	PG4	B	330	-	12,12,12	0.34	0	11,11,11	0.49	0
8	PG4	D	333	-	12,12,12	0.42	0	11,11,11	0.68	0
2	BEN	D	306[A]	-	9,9,9	0.68	0	7,11,11	0.78	0
5	PEG	B	326	-	6,6,6	0.29	0	5,5,5	0.69	0
5	PEG	D	324	-	6,6,6	0.27	0	5,5,5	0.33	0
5	PEG	B	308	-	6,6,6	0.26	0	5,5,5	0.30	0
5	PEG	B	319	-	6,6,6	0.22	0	5,5,5	0.25	0
3	PG5	C	306	-	11,11,11	0.32	0	10,10,10	0.30	0
8	PG4	B	328	-	12,12,12	0.28	0	11,11,11	0.25	0
7	MLI	B	321	-	6,6,6	1.73	1 (16%)	7,7,7	1.15	0
5	PEG	D	310	-	6,6,6	0.24	0	5,5,5	0.25	0
5	PEG	D	327	-	6,6,6	0.27	0	5,5,5	0.25	0
4	PG6	A	303	-	17,17,17	0.33	0	16,16,16	0.37	0
8	PG4	D	329	-	12,12,12	0.37	0	11,11,11	0.39	0
3	PG5	B	327	-	11,11,11	0.30	0	10,10,10	0.16	0
7	MLI	C	315	-	6,6,6	1.69	1 (16%)	7,7,7	1.18	0
8	PG4	A	318	-	12,12,12	0.28	0	11,11,11	0.38	0
7	MLI	A	311	-	6,6,6	1.78	1 (16%)	7,7,7	0.99	0
5	PEG	A	309	-	6,6,6	0.25	0	5,5,5	0.26	0
5	PEG	C	328[B]	-	6,6,6	0.27	0	5,5,5	0.26	0
5	PEG	A	313	-	6,6,6	0.29	0	5,5,5	0.42	0
5	PEG	B	324	-	6,6,6	0.28	0	5,5,5	0.15	0
2	BEN	A	301	-	9,9,9	0.51	0	7,11,11	0.35	0
5	PEG	A	314	-	6,6,6	0.24	0	5,5,5	0.32	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	PEG	C	328[A]	-	6,6,6	0.25	0	5,5,5	0.26	0
2	BEN	B	304	-	9,9,9	0.66	0	7,11,11	1.15	1 (14%)
5	PEG	C	312	-	6,6,6	0.26	0	5,5,5	0.73	0
5	PEG	D	311	-	6,6,6	0.29	0	5,5,5	0.25	0
5	PEG	A	312	-	6,6,6	0.24	0	5,5,5	0.24	0
3	PG5	A	304	-	11,11,11	0.28	0	10,10,10	0.27	0
5	PEG	D	307	-	6,6,6	0.24	0	5,5,5	0.25	0
5	PEG	D	319	-	6,6,6	0.23	0	5,5,5	0.44	0
5	PEG	D	326	-	6,6,6	0.22	0	5,5,5	0.16	0
5	PEG	A	306	-	6,6,6	0.25	0	5,5,5	0.22	0
10	EPE	C	303	-	15,15,15	0.87	1 (6%)	19,20,20	0.87	0
5	PEG	A	319	-	6,6,6	0.28	0	5,5,5	0.67	0
2	BEN	D	309	-	9,9,9	0.86	0	7,11,11	1.26	1 (14%)
3	PG5	D	312	-	11,11,11	0.35	0	10,10,10	0.87	0
5	PEG	B	316	-	6,6,6	0.25	0	5,5,5	0.30	0
5	PEG	B	323	-	6,6,6	0.28	0	5,5,5	0.53	0
5	PEG	D	336	-	6,6,6	0.25	0	5,5,5	0.17	0
8	PG4	B	329	-	12,12,12	0.43	0	11,11,11	0.93	0
8	PG4	A	315	-	11,11,12	0.28	0	10,10,11	0.81	1 (10%)
3	PG5	C	305	-	11,11,11	0.31	0	10,10,10	0.20	0
3	PG5	D	304	-	11,11,11	0.30	0	10,10,10	0.17	0
2	BEN	B	303	-	9,9,9	0.60	0	7,11,11	1.57	2 (28%)
5	PEG	D	322	2	6,6,6	0.36	0	5,5,5	0.51	0
5	PEG	C	316	-	6,6,6	0.26	0	5,5,5	0.46	0
2	BEN	B	301	-	9,9,9	0.55	0	7,11,11	1.97	3 (42%)
8	PG4	C	323	-	12,12,12	0.29	0	11,11,11	0.23	0
5	PEG	B	322	-	6,6,6	0.25	0	5,5,5	0.24	0
5	PEG	D	337	-	6,6,6	0.23	0	5,5,5	0.27	0
5	PEG	B	309	-	6,6,6	0.29	0	5,5,5	0.17	0
10	EPE	D	305	-	15,15,15	0.87	1 (6%)	19,20,20	1.17	2 (10%)
5	PEG	C	310	-	6,6,6	0.26	0	5,5,5	0.22	0
9	PMA	B	302	-	18,18,18	1.36	2 (11%)	26,26,26	1.55	5 (19%)
8	PG4	C	325	-	12,12,12	0.29	0	11,11,11	0.34	0
5	PEG	C	304	-	6,6,6	0.25	0	5,5,5	0.19	0
3	PG5	A	302	-	11,11,11	0.30	0	10,10,10	0.28	0
8	PG4	C	322	-	12,12,12	0.27	0	11,11,11	0.24	0
5	PEG	D	320	-	6,6,6	0.28	0	5,5,5	0.49	0
5	PEG	C	327	-	6,6,6	0.24	0	5,5,5	0.22	0
5	PEG	C	318	-	6,6,6	0.23	0	5,5,5	0.26	0
5	PEG	D	325	-	6,6,6	0.33	0	5,5,5	0.23	0
2	BEN	D	301	-	9,9,9	1.02	1 (11%)	7,11,11	1.92	3 (42%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	PEG	D	316	-	6,6,6	0.24	0	5,5,5	0.40	0
5	PEG	D	318[B]	-	6,6,6	0.25	0	5,5,5	0.23	0
5	PEG	D	317	-	6,6,6	0.32	0	5,5,5	0.47	0
5	PEG	C	313	-	6,6,6	0.26	0	5,5,5	0.28	0
8	PG4	A	316	-	12,12,12	0.32	0	11,11,11	0.45	0
3	PG5	B	305	-	11,11,11	0.42	0	10,10,10	0.70	0
5	PEG	B	317[B]	-	6,6,6	0.26	0	5,5,5	0.24	0
3	PG5	A	305	-	11,11,11	0.33	0	10,10,10	0.20	0
7	MLI	D	315	-	6,6,6	1.54	1 (16%)	7,7,7	1.18	0
5	PEG	C	317	-	6,6,6	0.26	0	5,5,5	0.24	0
5	PEG	A	308	-	6,6,6	0.24	0	5,5,5	0.18	0
3	PG5	D	303	-	11,11,11	0.29	0	10,10,10	0.18	0
5	PEG	C	320	-	6,6,6	0.27	0	5,5,5	0.46	0
5	PEG	C	311	-	6,6,6	0.27	0	5,5,5	0.20	0
5	PEG	B	314	-	6,6,6	0.24	0	5,5,5	0.32	0
5	PEG	D	318[A]	-	6,6,6	0.25	0	5,5,5	0.44	0
8	PG4	D	331	-	12,12,12	0.29	0	11,11,11	0.23	0
5	PEG	B	317[A]	-	6,6,6	0.25	0	5,5,5	0.29	0
5	PEG	C	319	-	6,6,6	0.23	0	5,5,5	0.26	0
2	BEN	C	307	-	9,9,9	0.64	0	7,11,11	0.99	1 (14%)
8	PG4	D	330	-	12,12,12	0.30	0	11,11,11	0.25	0
5	PEG	D	323	-	6,6,6	0.27	0	5,5,5	0.36	0
5	PEG	B	331	-	6,6,6	0.24	0	5,5,5	0.23	0
5	PEG	C	308	-	6,6,6	0.52	0	5,5,5	1.10	1 (20%)
5	PEG	B	310	-	6,6,6	0.24	0	5,5,5	0.19	0
5	PEG	B	318	-	6,6,6	0.28	0	5,5,5	0.19	0
8	PG4	D	328	-	12,12,12	0.30	0	11,11,11	0.26	0
5	PEG	D	335	-	6,6,6	0.30	0	5,5,5	0.39	0
5	PEG	B	315	-	6,6,6	0.25	0	5,5,5	0.25	0
2	BEN	C	302	-	9,9,9	0.72	0	7,11,11	2.00	2 (28%)
5	PEG	C	321	-	6,6,6	0.23	0	5,5,5	0.22	0
5	PEG	A	307	-	6,6,6	0.27	0	5,5,5	0.28	0
8	PG4	A	317	-	12,12,12	0.34	0	11,11,11	0.26	0
2	BEN	C	301	-	9,9,9	0.71	0	7,11,11	1.29	1 (14%)
5	PEG	B	313	-	6,6,6	0.25	0	5,5,5	0.24	0
3	PG5	B	311	-	11,11,11	0.31	0	10,10,10	0.25	0
5	PEG	B	325	-	6,6,6	0.29	0	5,5,5	0.31	0
5	PEG	D	321	-	6,6,6	0.30	0	5,5,5	0.40	0
8	PG4	C	324	-	12,12,12	0.35	0	11,11,11	0.48	0
8	PG4	C	326	-	12,12,12	0.26	0	11,11,11	0.24	0
9	PMA	D	302	-	18,18,18	1.25	3 (16%)	26,26,26	1.52	4 (15%)
8	PG4	D	332	-	12,12,12	0.29	0	11,11,11	0.24	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	PEG	C	309	-	6,6,6	0.28	0	5,5,5	0.48	0
2	BEN	D	306[B]	5	9,9,9	1.40	1 (11%)	7,11,11	1.88	2 (28%)
5	PEG	B	306	-	6,6,6	0.22	0	5,5,5	0.34	0
5	PEG	B	312	-	6,6,6	0.29	0	5,5,5	0.19	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	D	308	-	-	2/4/4/4	-
5	PEG	D	334	-	-	3/4/4/4	-
3	PG5	B	307	-	-	3/9/9/9	-
8	PG4	B	330	-	-	6/10/10/10	-
8	PG4	D	333	-	-	5/10/10/10	-
2	BEN	D	306[A]	-	-	0/4/4/4	0/1/1/1
5	PEG	B	326	-	-	3/4/4/4	-
5	PEG	D	324	-	-	3/4/4/4	-
5	PEG	B	308	-	-	1/4/4/4	-
5	PEG	B	319	-	-	2/4/4/4	-
3	PG5	C	306	-	-	5/9/9/9	-
8	PG4	B	328	-	-	7/10/10/10	-
7	MLI	B	321	-	-	3/4/4/4	-
5	PEG	D	310	-	-	0/4/4/4	-
5	PEG	D	327	-	-	3/4/4/4	-
4	PG6	A	303	-	-	7/15/15/15	-
8	PG4	D	329	-	-	3/10/10/10	-
3	PG5	B	327	-	-	5/9/9/9	-
7	MLI	C	315	-	-	2/4/4/4	-
8	PG4	A	318	-	-	5/10/10/10	-
7	MLI	A	311	-	-	4/4/4/4	-
5	PEG	A	309	-	-	2/4/4/4	-
5	PEG	C	328[B]	-	-	1/4/4/4	-
5	PEG	A	313	-	-	3/4/4/4	-
5	PEG	B	324	-	-	2/4/4/4	-
2	BEN	A	301	-	-	0/4/4/4	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	PEG	A	314	-	-	1/4/4/4	-
5	PEG	C	328[A]	-	-	1/4/4/4	-
2	BEN	B	304	-	-	4/4/4/4	0/1/1/1
5	PEG	C	312	-	-	3/4/4/4	-
5	PEG	D	311	-	-	3/4/4/4	-
5	PEG	A	312	-	-	3/4/4/4	-
3	PG5	A	304	-	-	4/9/9/9	-
5	PEG	D	307	-	-	1/4/4/4	-
5	PEG	D	319	-	-	3/4/4/4	-
5	PEG	D	326	-	-	3/4/4/4	-
5	PEG	A	306	-	-	3/4/4/4	-
10	EPE	C	303	-	-	3/9/19/19	0/1/1/1
5	PEG	A	319	-	-	1/4/4/4	-
2	BEN	D	309	-	-	2/4/4/4	0/1/1/1
3	PG5	D	312	-	-	7/9/9/9	-
5	PEG	B	316	-	-	3/4/4/4	-
5	PEG	B	323	-	-	1/4/4/4	-
5	PEG	D	336	-	-	4/4/4/4	-
8	PG4	B	329	-	-	5/10/10/10	-
8	PG4	A	315	-	-	2/9/9/10	-
3	PG5	C	305	-	-	6/9/9/9	-
3	PG5	D	304	-	-	5/9/9/9	-
2	BEN	B	303	-	-	0/4/4/4	0/1/1/1
5	PEG	D	322	2	-	2/4/4/4	-
5	PEG	C	316	-	-	2/4/4/4	-
2	BEN	B	301	-	-	2/4/4/4	0/1/1/1
8	PG4	C	323	-	-	5/10/10/10	-
5	PEG	B	322	-	-	3/4/4/4	-
5	PEG	D	337	-	-	1/4/4/4	-
5	PEG	B	309	-	-	2/4/4/4	-
10	EPE	D	305	-	-	4/9/19/19	0/1/1/1
5	PEG	C	310	-	-	1/4/4/4	-
9	PMA	B	302	-	-	6/16/16/16	0/1/1/1
8	PG4	C	325	-	-	6/10/10/10	-
5	PEG	C	304	-	-	1/4/4/4	-
3	PG5	A	302	-	-	5/9/9/9	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	PG4	C	322	-	-	5/10/10/10	-
5	PEG	D	320	-	-	2/4/4/4	-
5	PEG	C	327	-	-	2/4/4/4	-
5	PEG	C	318	-	-	0/4/4/4	-
5	PEG	D	325	-	-	1/4/4/4	-
2	BEN	D	301	-	-	0/4/4/4	0/1/1/1
5	PEG	D	316	-	-	2/4/4/4	-
5	PEG	D	318[B]	-	-	2/4/4/4	-
5	PEG	D	317	-	-	2/4/4/4	-
5	PEG	C	313	-	-	3/4/4/4	-
8	PG4	A	316	-	-	7/10/10/10	-
3	PG5	B	305	-	-	5/9/9/9	-
5	PEG	B	317[B]	-	-	1/4/4/4	-
3	PG5	A	305	-	-	6/9/9/9	-
7	MLI	D	315	-	-	0/4/4/4	-
5	PEG	C	317	-	-	2/4/4/4	-
5	PEG	A	308	-	-	2/4/4/4	-
3	PG5	D	303	-	-	4/9/9/9	-
5	PEG	C	320	-	-	2/4/4/4	-
5	PEG	C	311	-	-	2/4/4/4	-
5	PEG	B	314	-	-	3/4/4/4	-
5	PEG	D	318[A]	-	-	2/4/4/4	-
8	PG4	D	331	-	-	4/10/10/10	-
5	PEG	B	317[A]	-	-	1/4/4/4	-
5	PEG	C	319	-	-	4/4/4/4	-
2	BEN	C	307	-	-	3/4/4/4	0/1/1/1
8	PG4	D	330	-	-	7/10/10/10	-
5	PEG	D	323	-	-	2/4/4/4	-
5	PEG	B	331	-	-	1/4/4/4	-
5	PEG	C	308	-	-	4/4/4/4	-
5	PEG	B	310	-	-	1/4/4/4	-
5	PEG	B	318	-	-	2/4/4/4	-
8	PG4	D	328	-	-	4/10/10/10	-
5	PEG	D	335	-	-	3/4/4/4	-
5	PEG	B	315	-	-	2/4/4/4	-
2	BEN	C	302	-	-	0/4/4/4	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	PEG	C	321	-	-	3/4/4/4	-
5	PEG	A	307	-	-	1/4/4/4	-
8	PG4	A	317	-	-	7/10/10/10	-
2	BEN	C	301	-	-	0/4/4/4	0/1/1/1
5	PEG	B	313	-	-	2/4/4/4	-
3	PG5	B	311	-	-	6/9/9/9	-
5	PEG	B	325	-	-	2/4/4/4	-
5	PEG	D	321	-	-	2/4/4/4	-
8	PG4	C	324	-	-	5/10/10/10	-
8	PG4	C	326	-	-	3/10/10/10	-
9	PMA	D	302	-	-	2/16/16/16	0/1/1/1
8	PG4	D	332	-	-	6/10/10/10	-
5	PEG	C	309	-	-	2/4/4/4	-
2	BEN	D	306[B]	5	-	0/4/4/4	0/1/1/1
5	PEG	B	306	-	-	2/4/4/4	-
5	PEG	B	312	-	-	3/4/4/4	-

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	306[B]	BEN	C6-C1	3.27	1.44	1.39
7	B	321	MLI	C1-C3	2.83	1.55	1.51
7	A	311	MLI	C1-C3	2.81	1.55	1.51
7	C	315	MLI	C1-C3	2.71	1.55	1.51
9	B	302	PMA	C2-C10	2.51	1.55	1.49

The worst 5 of 29 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	D	302	PMA	O5-C7-C4	-4.64	110.90	121.97
9	B	302	PMA	O7-C8-C5	-3.73	113.07	121.97
2	D	306[B]	BEN	C1-C-N2	-3.36	112.92	118.01
2	B	301	BEN	C5-C6-C1	3.32	123.62	120.36
2	D	309	BEN	C1-C-N2	-3.28	113.03	118.01

There are no chirality outliers.

5 of 327 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	309	BEN	N2-C-C1-C2
2	D	309	BEN	N2-C-C1-C6
10	C	303	EPE	C8-C7-N4-C5
10	D	305	EPE	N4-C7-C8-O8
3	B	327	PG5	O3-C6-C7-O4

There are no ring outliers.

74 monomers are involved in 159 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	308	PEG	1	0
3	B	307	PG5	1	0
8	B	330	PG4	4	0
8	D	333	PG4	7	2
5	D	324	PEG	1	0
5	B	308	PEG	2	0
5	B	319	PEG	2	0
3	C	306	PG5	3	0
7	B	321	MLI	1	0
5	D	310	PEG	1	0
5	D	327	PEG	1	0
4	A	303	PG6	2	0
8	D	329	PG4	4	0
8	A	318	PG4	1	0
7	A	311	MLI	1	0
5	B	324	PEG	1	0
5	C	328[A]	PEG	1	0
2	B	304	BEN	2	0
5	C	312	PEG	4	0
5	D	311	PEG	1	0
3	A	304	PG5	2	0
5	D	319	PEG	6	0
5	A	306	PEG	1	0
10	C	303	EPE	3	0
2	D	309	BEN	1	0
3	D	312	PG5	4	0
5	B	316	PEG	3	0
5	D	336	PEG	1	0
8	B	329	PG4	3	0
8	A	315	PG4	0	1
3	C	305	PG5	1	0
3	D	304	PG5	1	0
2	B	303	BEN	1	0

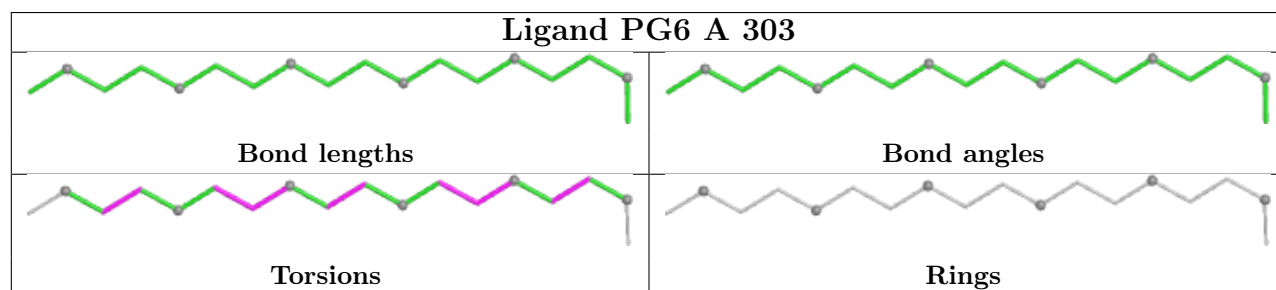
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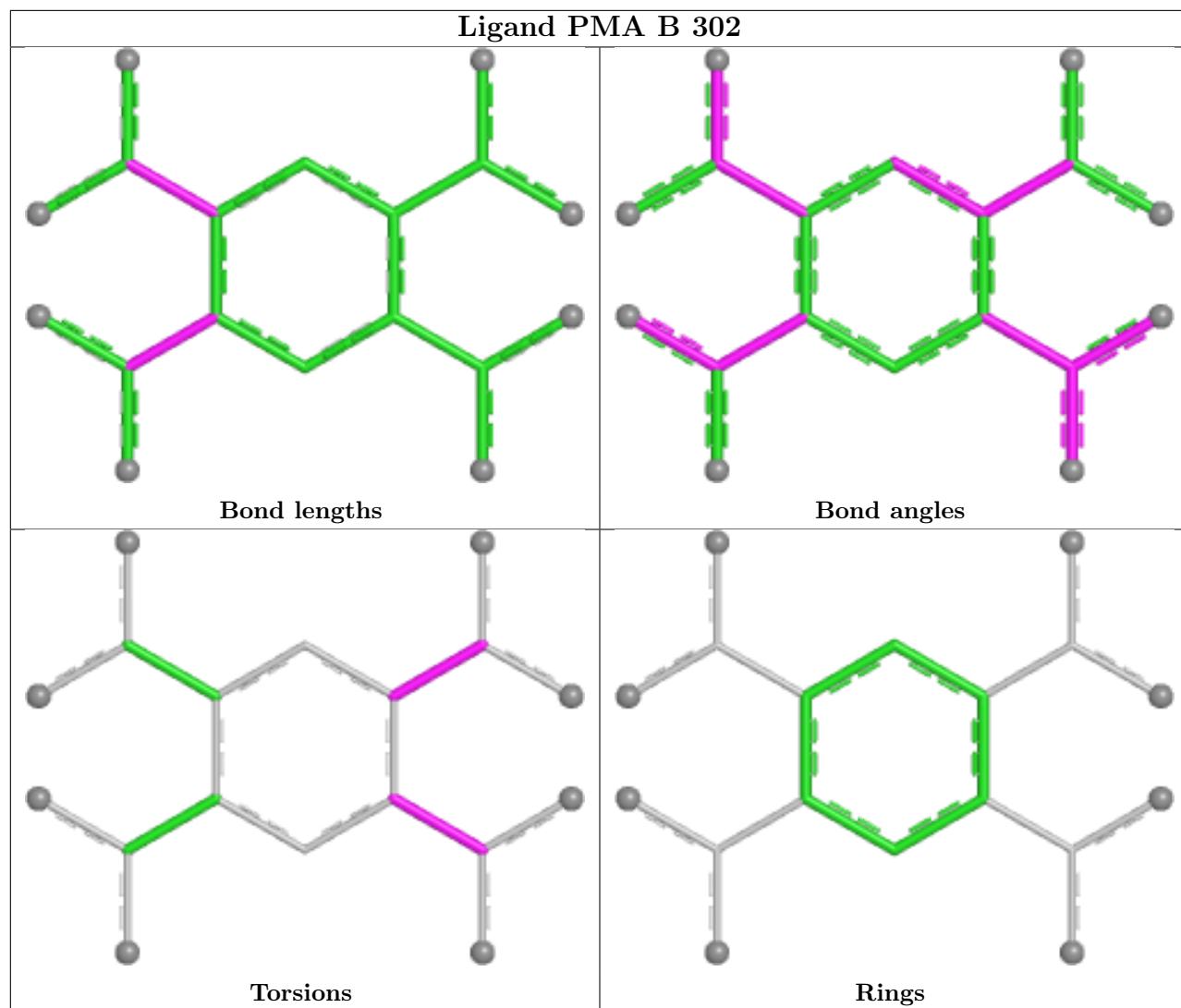
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	322	PEG	3	0
5	C	316	PEG	4	0
5	B	322	PEG	1	0
5	D	337	PEG	1	0
5	B	309	PEG	3	0
10	D	305	EPE	3	0
9	B	302	PMA	3	0
8	C	325	PG4	5	0
3	A	302	PG5	2	0
8	C	322	PG4	1	0
5	D	320	PEG	9	0
5	D	316	PEG	1	0
5	D	318[B]	PEG	1	0
5	D	317	PEG	3	0
5	C	313	PEG	1	0
8	A	316	PG4	1	1
3	B	305	PG5	3	0
5	B	317[B]	PEG	3	0
3	A	305	PG5	2	0
3	D	303	PG5	4	0
5	C	320	PEG	1	0
5	D	318[A]	PEG	2	0
8	D	331	PG4	1	0
5	B	317[A]	PEG	3	0
8	D	330	PG4	2	0
5	C	308	PEG	10	0
8	D	328	PG4	0	1
5	D	335	PEG	2	0
5	A	307	PEG	2	0
8	A	317	PG4	1	0
2	C	301	BEN	4	0
3	B	311	PG5	4	0
5	B	325	PEG	4	0
5	D	321	PEG	3	1
8	C	324	PG4	3	0
8	C	326	PG4	2	0
9	D	302	PMA	4	0
8	D	332	PG4	0	1
5	C	309	PEG	5	0
5	B	306	PEG	1	0
5	B	312	PEG	1	0

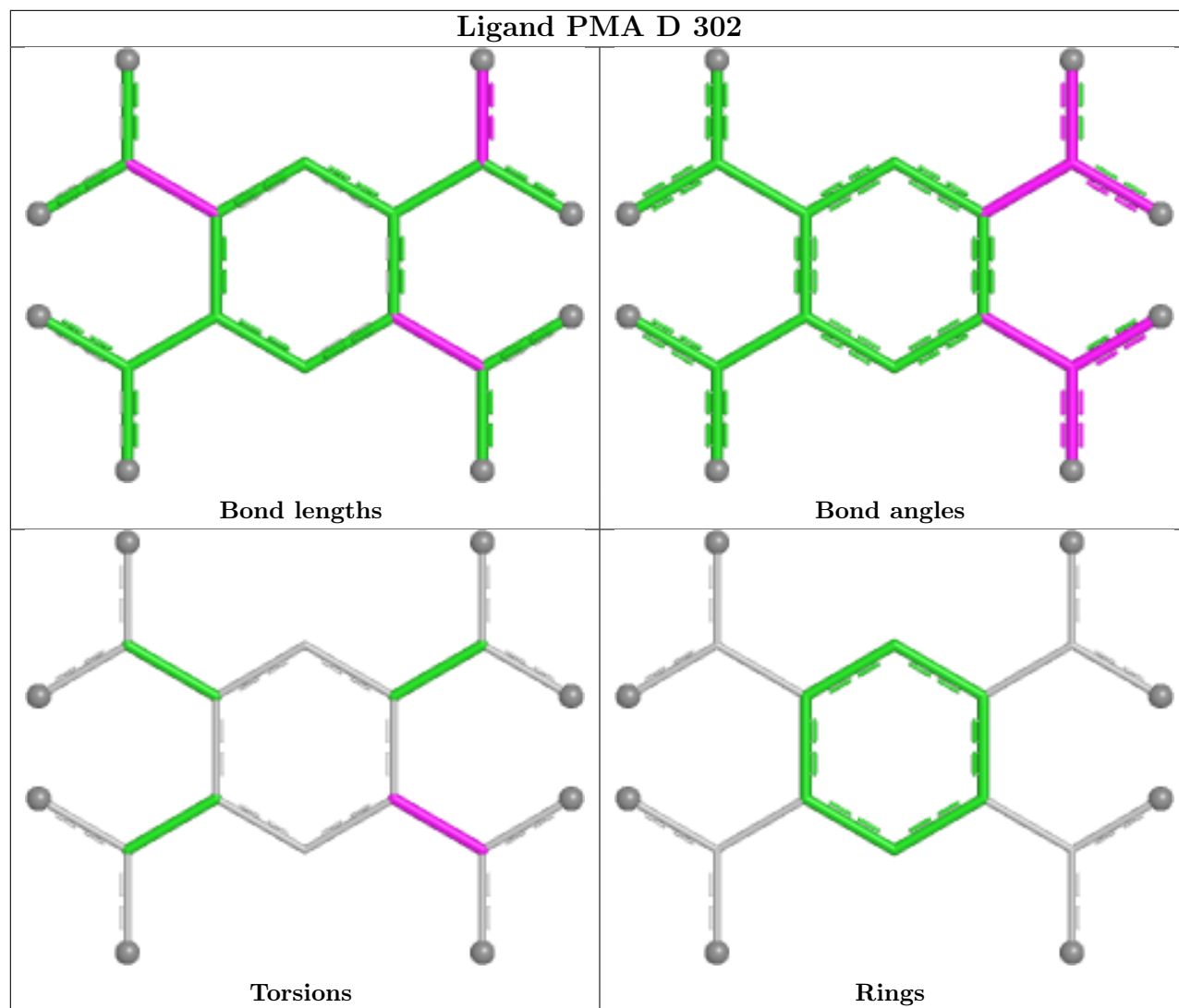
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

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	223/231 (96%)	1.04	27 (12%)	10 11	15, 21, 31, 38	3 (1%)
1	B	223/231 (96%)	1.31	43 (19%)	4 4	18, 29, 47, 51	2 (0%)
1	C	223/231 (96%)	1.06	30 (13%)	8 8	14, 19, 27, 34	1 (0%)
1	D	223/231 (96%)	0.74	9 (4%)	43 45	10, 18, 32, 47	6 (2%)
All	All	892/924 (96%)	1.04	109 (12%)	10 11	10, 21, 38, 51	12 (1%)

The worst 5 of 109 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	163	CYS	6.1
1	B	212	CYS	4.9
1	B	73	LEU	4.8
1	C	218	PRO	3.9
1	B	114	ARG	3.9

### 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( $\text{\AA}^2$ )	Q<0.9
7	MLI	A	311	7/7	0.39	0.15	48,72,86,91	0
5	PEG	D	322	7/7	0.40	0.17	52,63,71,71	17
5	PEG	D	318[A]	7/7	0.45	0.20	30,55,66,66	17
5	PEG	D	318[B]	7/7	0.45	0.20	37,53,67,72	17
5	PEG	C	328[A]	7/7	0.45	0.24	42,57,69,69	17
5	PEG	C	328[B]	7/7	0.45	0.24	46,60,72,74	17
8	PG4	B	330	13/13	0.47	0.21	35,57,74,77	31
5	PEG	D	319	7/7	0.50	0.21	46,57,69,71	16
5	PEG	D	327	7/7	0.51	0.13	52,65,81,84	0
5	PEG	B	317[A]	7/7	0.51	0.15	38,60,72,72	17
5	PEG	B	317[B]	7/7	0.51	0.15	49,59,69,69	17
5	PEG	C	309	7/7	0.53	0.20	25,57,68,78	17
5	PEG	B	322	7/7	0.55	0.18	42,59,67,77	17
8	PG4	C	325	13/13	0.55	0.20	32,57,68,71	31
5	PEG	C	320	7/7	0.56	0.18	34,54,65,65	17
7	MLI	C	315	7/7	0.56	0.19	30,62,71,73	9
8	PG4	A	317	13/13	0.56	0.20	25,59,77,78	31
5	PEG	D	326	7/7	0.56	0.20	44,57,69,69	17
3	PG5	D	304	12/12	0.56	0.16	38,64,73,78	30
8	PG4	C	323	13/13	0.58	0.17	47,60,66,68	31
3	PG5	B	327	12/12	0.58	0.19	48,60,66,66	30
3	PG5	B	307	12/12	0.59	0.21	22,46,66,66	30
5	PEG	C	308	7/7	0.59	0.19	31,62,79,91	0
2	BEN	C	307	9/9	0.60	0.15	45,63,87,87	0
5	PEG	D	308	7/7	0.60	0.24	26,54,64,67	17
8	PG4	D	331	13/13	0.60	0.18	42,56,69,71	31
8	PG4	D	332	13/13	0.60	0.17	44,54,64,64	31
7	MLI	B	321	7/7	0.61	0.11	55,64,74,75	0
5	PEG	B	324	7/7	0.61	0.20	28,53,77,77	17
5	PEG	D	324	7/7	0.62	0.25	21,56,69,75	17
5	PEG	A	308	7/7	0.62	0.16	53,64,71,75	0
7	MLI	D	315	7/7	0.62	0.15	37,47,49,59	9
3	PG5	C	306	12/12	0.63	0.24	41,52,63,63	30
8	PG4	C	322	13/13	0.63	0.17	45,55,67,67	31
8	PG4	B	328	13/13	0.63	0.18	43,58,66,68	31
3	PG5	B	311	12/12	0.64	0.16	30,52,60,60	30
5	PEG	D	321	7/7	0.64	0.17	29,49,68,68	17
3	PG5	D	303	12/12	0.64	0.26	21,36,59,59	29
5	PEG	D	316	7/7	0.65	0.16	48,58,70,70	17
5	PEG	B	325	7/7	0.66	0.23	36,58,67,67	17
8	PG4	D	330	13/13	0.66	0.22	35,59,71,74	31
4	PG6	A	303	18/18	0.66	0.18	23,54,67,74	44
5	PEG	D	337	7/7	0.66	0.21	45,54,61,61	17

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	PEG	B	318	7/7	0.67	0.21	33,51,62,62	17
5	PEG	B	308	7/7	0.67	0.18	34,56,78,78	17
3	PG5	C	305	12/12	0.67	0.18	33,60,73,84	30
5	PEG	C	321	7/7	0.67	0.12	47,56,67,69	17
3	PG5	A	304	12/12	0.67	0.20	32,56,63,72	30
5	PEG	C	317	7/7	0.68	0.19	32,50,60,60	17
5	PEG	D	335	7/7	0.68	0.18	28,46,66,79	17
5	PEG	C	318	7/7	0.68	0.15	47,56,68,68	17
3	PG5	A	302	12/12	0.68	0.18	29,52,66,70	30
10	EPE	C	303	15/15	0.68	0.17	27,49,61,64	31
5	PEG	D	310	7/7	0.69	0.20	29,47,60,60	17
5	PEG	A	307	7/7	0.69	0.24	38,59,71,75	17
5	PEG	B	331	7/7	0.69	0.12	48,57,61,63	17
5	PEG	C	327	7/7	0.69	0.18	34,53,64,64	17
8	PG4	A	316	13/13	0.69	0.16	37,57,68,79	30
5	PEG	B	314	7/7	0.70	0.15	53,63,66,67	17
5	PEG	B	316	7/7	0.70	0.14	49,63,76,79	17
3	PG5	D	312	12/12	0.71	0.27	23,53,73,76	30
8	PG4	D	329	13/13	0.71	0.20	20,53,65,67	31
3	PG5	A	305	12/12	0.71	0.17	28,51,62,68	30
8	PG4	C	326	13/13	0.72	0.24	34,53,62,63	31
5	PEG	B	319	7/7	0.72	0.21	26,48,60,60	17
5	PEG	C	304	7/7	0.72	0.22	27,58,70,71	17
2	BEN	D	309	9/9	0.72	0.16	27,63,80,81	0
5	PEG	A	306	7/7	0.72	0.17	40,55,66,66	17
5	PEG	A	314	7/7	0.72	0.15	32,51,76,76	0
5	PEG	B	326	7/7	0.73	0.17	40,50,65,67	16
5	PEG	B	312	7/7	0.73	0.14	31,49,67,67	17
5	PEG	D	323	7/7	0.73	0.16	31,58,66,67	17
5	PEG	C	310	7/7	0.73	0.15	27,60,73,73	17
5	PEG	A	309	7/7	0.73	0.16	38,50,62,65	17
5	PEG	B	313	7/7	0.74	0.14	35,58,70,70	17
5	PEG	D	311	7/7	0.75	0.22	19,48,66,66	17
8	PG4	A	318	13/13	0.75	0.21	24,53,65,76	31
5	PEG	D	320	7/7	0.75	0.16	47,58,65,72	15
5	PEG	C	319	7/7	0.75	0.22	22,52,63,63	17
8	PG4	D	328	13/13	0.75	0.22	35,55,65,74	31
8	PG4	A	315	12/13	0.76	0.28	27,52,59,64	29
5	PEG	D	317	7/7	0.76	0.13	29,50,70,70	0
5	PEG	A	312	7/7	0.77	0.14	42,56,64,64	17
8	PG4	B	329	13/13	0.78	0.25	17,48,67,68	31
5	PEG	B	306	7/7	0.78	0.17	29,45,73,73	17

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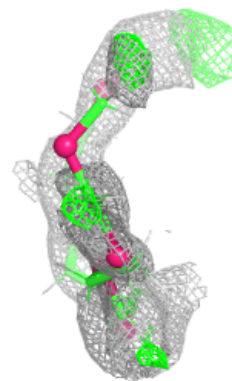
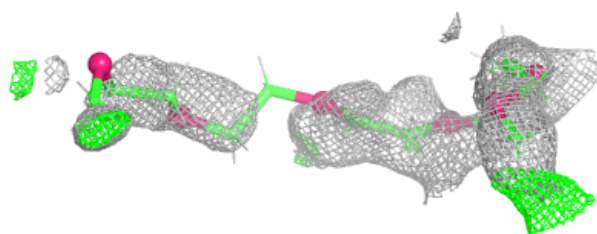
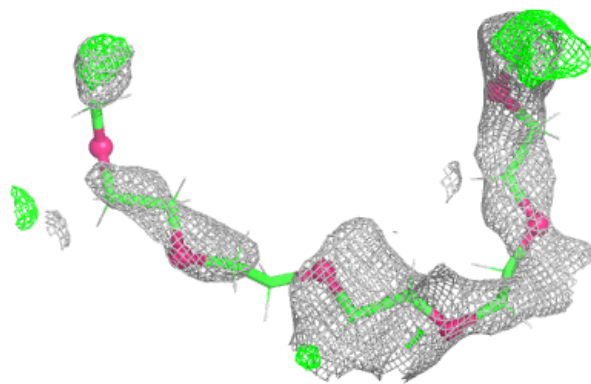
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	BEN	D	306[A]	9/9	0.78	0.17	37,52,66,73	17
2	BEN	D	306[B]	9/9	0.78	0.17	34,49,74,74	17
5	PEG	D	307	7/7	0.78	0.21	41,57,76,76	17
3	PG5	B	305	12/12	0.78	0.22	23,45,70,78	30
8	PG4	C	324	13/13	0.79	0.15	27,57,73,77	31
5	PEG	C	312	7/7	0.79	0.15	30,58,70,78	17
5	PEG	B	310	7/7	0.79	0.12	37,57,69,78	17
10	EPE	D	305	15/15	0.79	0.16	27,54,80,83	32
8	PG4	D	333	13/13	0.80	0.26	24,53,64,70	31
5	PEG	D	325	7/7	0.80	0.14	25,51,83,83	17
5	PEG	B	323	7/7	0.80	0.16	17,55,69,70	17
2	BEN	B	304	9/9	0.81	0.28	37,54,73,80	17
5	PEG	A	319	7/7	0.81	0.17	31,50,77,77	17
5	PEG	D	334	7/7	0.81	0.16	25,54,69,69	17
5	PEG	B	315	7/7	0.81	0.12	46,56,67,68	17
5	PEG	D	336	7/7	0.81	0.17	23,46,64,64	17
5	PEG	C	311	7/7	0.83	0.18	20,50,67,67	17
5	PEG	A	313	7/7	0.84	0.19	22,39,58,58	17
2	BEN	C	301	9/9	0.84	0.11	17,22,26,28	0
5	PEG	C	316	7/7	0.85	0.16	32,54,64,65	17
5	PEG	B	309	7/7	0.85	0.20	22,33,50,60	17
5	PEG	C	313	7/7	0.85	0.12	23,52,66,66	17
2	BEN	A	301	9/9	0.88	0.09	18,23,29,30	0
9	PMA	B	302	18/18	0.90	0.09	23,29,50,74	0
2	BEN	B	301	9/9	0.93	0.10	20,25,30,33	0
2	BEN	B	303	9/9	0.93	0.08	19,24,32,32	0
2	BEN	D	301	9/9	0.94	0.08	17,22,26,26	0
9	PMA	D	302	18/18	0.94	0.07	15,16,23,25	0
6	CA	B	320	1/1	0.94	0.07	37,37,37,37	0
2	BEN	C	302	9/9	0.94	0.08	15,19,26,27	0
11	CL	D	338	1/1	0.94	0.15	25,25,25,25	0
6	CA	D	314	1/1	0.96	0.21	32,32,32,32	0
6	CA	D	313	1/1	0.96	0.05	20,20,20,20	0
6	CA	C	314	1/1	0.97	0.05	15,15,15,15	0
6	CA	A	310	1/1	0.97	0.05	19,19,19,19	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.

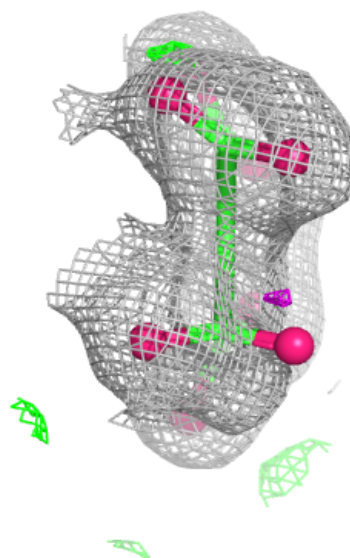
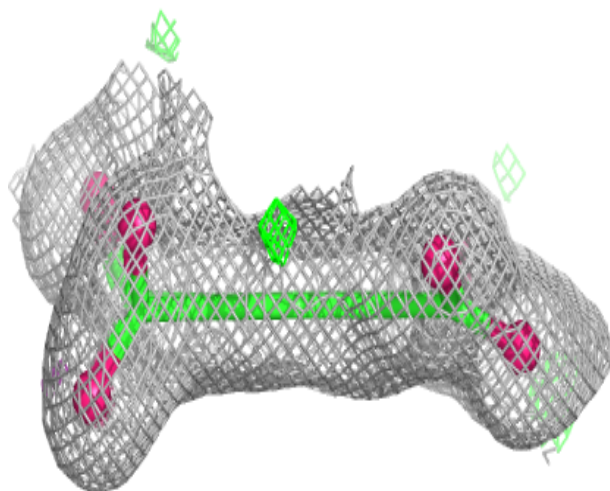
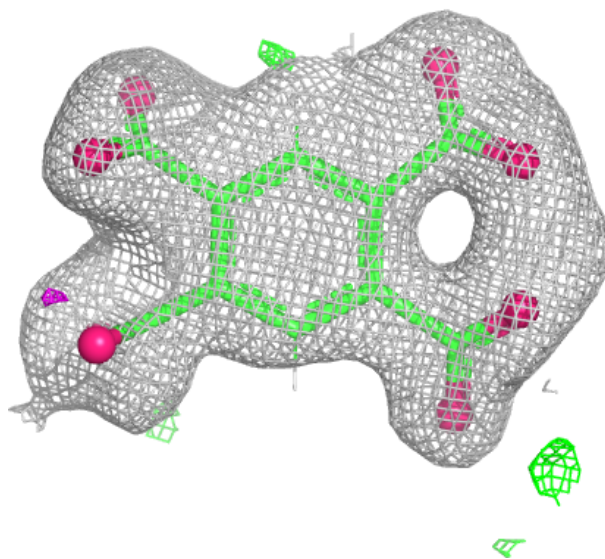
**Electron density around PG6 A 303:**

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

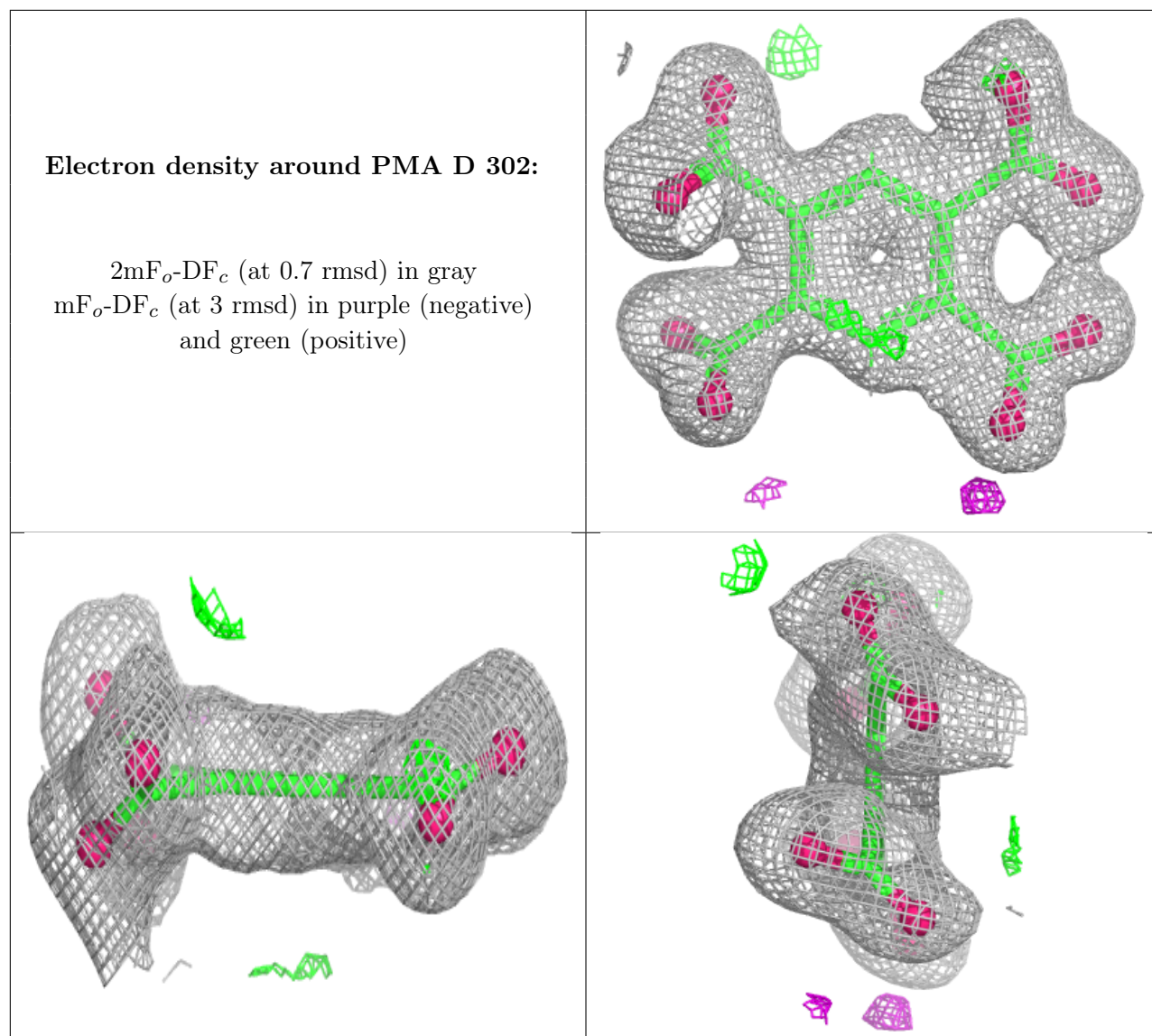


**Electron density around PMA B 302:**

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







## 6.5 Other polymers ⓘ

There are no such residues in this entry.