



# Full wwPDB EM Validation Report ⓘ

Oct 7, 2024 – 02:31 PM JST

PDB ID : 8ZOY  
EMDB ID : EMD-60322  
Title : Cryo-EM structure of human norepinephrine transporter NET bound with norepinephrine in an inward open state at a resolution of 2.5 angstrom  
Authors : Song, A.L.; Wu, X.D.  
Deposited on : 2024-05-29  
Resolution : 2.50 Å(reported)

This is a Full wwPDB EM Validation 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/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

---

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

EMDB validation analysis : **FAILED**  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : **FAILED**  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.39

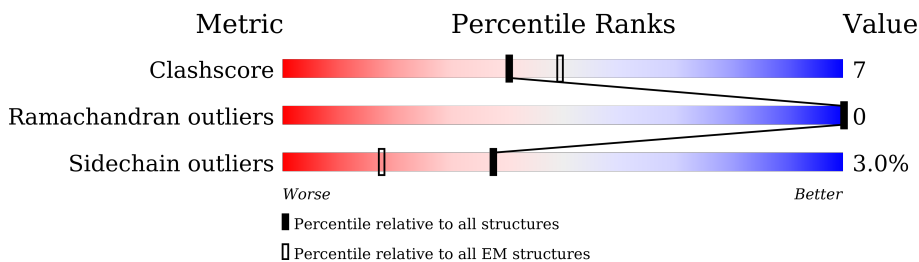
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.50 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)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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  $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	571	
2	B	120	

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 10745 atoms, of which 5304 are hydrogens and 0 are deuteriums.

In the tables below, 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.

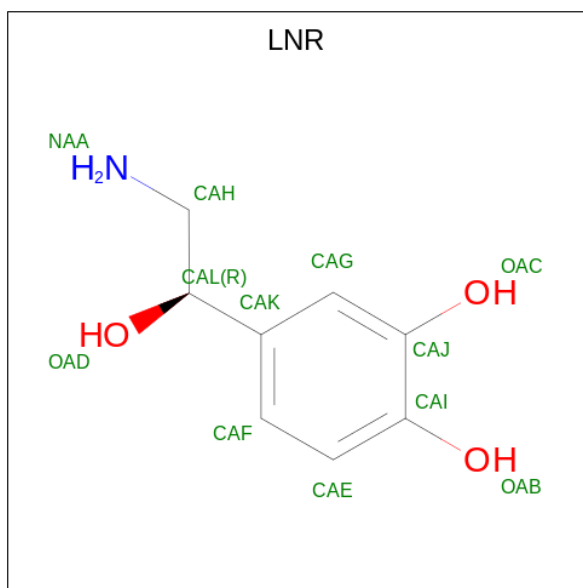
- Molecule 1 is a protein called Sodium-dependent noradrenaline transporter.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
1	A	547	8768	2953	4375	681	739	20	1	0

- Molecule 2 is a protein called Nb\_BF9.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
2	B	119	1822	589	885	160	184	4	0	0

- Molecule 3 is L-NOREPINEPHRINE (three-letter code: LNR) (formula: C<sub>8</sub>H<sub>11</sub>NO<sub>3</sub>).

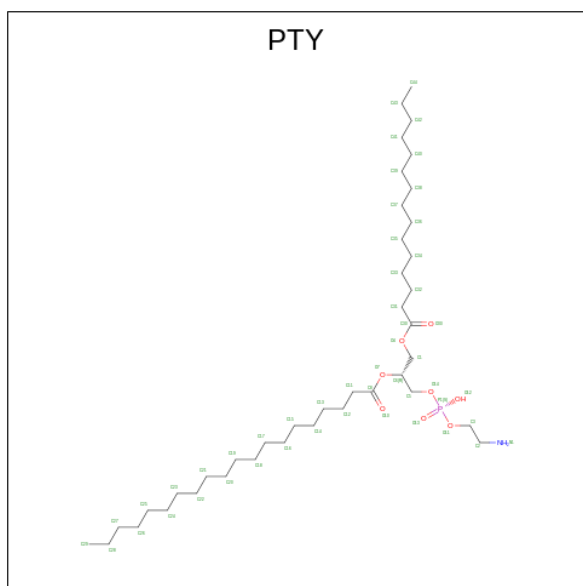


Mol	Chain	Residues	Atoms					AltConf
			Total	C	H	N	O	
3	A	1	23	8	11	1	3	0

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	AltConf
4	A	1	Total Cl 1 1	0

- Molecule 5 is PHOSPHATIDYLETHANOLAMINE (three-letter code: PTY) (formula:  $C_{40}H_{80}NO_8P$ ).



Mol	Chain	Residues	Atoms					AltConf	
			Total	C	H	N	O		P
5	A	1	61	18	33	1	8	1	0

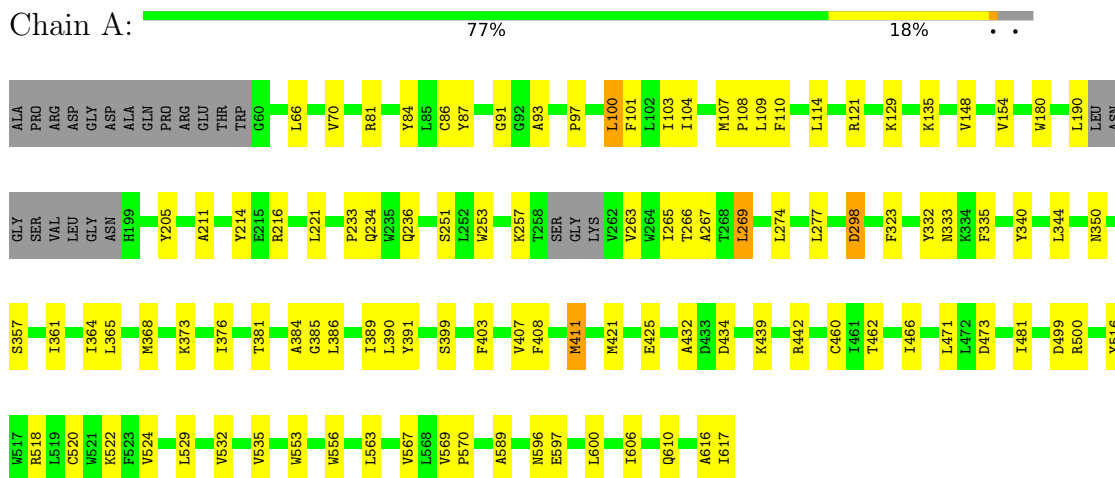
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	AltConf
6	A	62	Total O 62 62	0
6	B	8	Total O 8 8	0

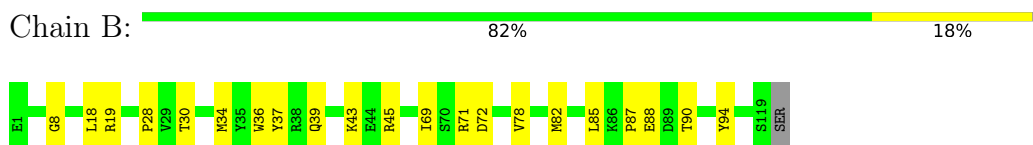
### 3 Residue-property plots

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. 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. 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: Sodium-dependent noradrenaline transporter



- Molecule 2: Nb\_BF9



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	612638	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor

## 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: PTY, CL, LNR

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	0.33	0/4536	0.47	0/6185
2	B	0.36	0/959	0.53	0/1302
All	All	0.34	0/5495	0.48	0/7487

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	4393	4375	4374	63	0
2	B	937	885	885	11	0
3	A	12	11	11	0	0
4	A	1	0	0	0	0
5	A	28	33	29	1	0
6	A	62	0	0	3	0
6	B	8	0	0	1	0
All	All	5441	5304	5299	72	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 7.

All (72) 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:439:LYS:HE2	6:A:855:HOH:O	1.90	0.71
1:A:135:LYS:NZ	1:A:434:ASP:OD2	2.21	0.71
1:A:84:TYR:OH	1:A:473:ASP:OD2	2.08	0.71
2:B:39:GLN:NE2	2:B:43:LYS:O	2.24	0.70
1:A:129:LYS:NZ	6:A:804:HOH:O	2.26	0.68
1:A:154:VAL:HG21	1:A:460:CYS:HB2	1.80	0.62
1:A:298:ASP:OD1	1:A:298:ASP:N	2.30	0.62
1:A:257:LYS:HG3	1:A:421:MET:HB3	1.83	0.61
1:A:234:GLN:NE2	1:A:236:GLN:OE1	2.33	0.60
1:A:522:LYS:NZ	1:A:616:ALA:O	2.35	0.56
1:A:364:ILE:O	1:A:368:MET:HG3	2.05	0.56
2:B:88:GLU:N	2:B:88:GLU:OE2	2.39	0.55
1:A:66:LEU:O	1:A:70:VAL:HG22	2.07	0.55
1:A:70:VAL:HG23	1:A:267:ALA:HB1	1.89	0.54
1:A:221:LEU:HD13	1:A:466:ILE:HG22	1.90	0.54
1:A:518:ARG:NH1	1:A:617:ILE:O	2.39	0.54
1:A:109:LEU:CD1	1:A:529:LEU:HD11	2.41	0.50
1:A:597:GLU:HB3	1:A:600:LEU:HD12	1.94	0.49
1:A:391:TYR:CD2	1:A:408:PHE:CZ	3.01	0.49
1:A:499:ASP:OD1	1:A:500:ARG:N	2.47	0.48
1:A:109:LEU:HD11	1:A:529:LEU:HD11	1.96	0.48
1:A:277:LEU:HD13	1:A:391:TYR:CE1	2.49	0.48
1:A:340:TYR:CZ	1:A:344:LEU:HD11	2.50	0.47
1:A:233:PRO:HA	1:A:462:THR:HA	1.97	0.47
1:A:596:ASN:ND2	2:B:30:THR:OG1	2.47	0.46
2:B:8:GLY:O	2:B:18:LEU:HD22	2.16	0.46
1:A:589:ALA:HB1	1:A:606:ILE:HG12	1.97	0.46
1:A:434:ASP:O	5:A:703:PTY:N1	2.49	0.46
1:A:148:VAL:HG21	1:A:323:PHE:HE1	1.81	0.46
1:A:180:TRP:O	1:A:216:ARG:NE	2.46	0.46
2:B:82:MET:HB3	2:B:85:LEU:HD21	1.97	0.45
1:A:569:VAL:HB	1:A:570:PRO:CD	2.47	0.45
1:A:263:VAL:O	1:A:267:ALA:HB3	2.16	0.45
1:A:265:ILE:HG23	1:A:266:THR:N	2.32	0.45
1:A:335:PHE:CZ	2:B:28:PRO:HD3	2.51	0.45
1:A:107:MET:HB3	1:A:108:PRO:HD3	1.98	0.44
1:A:269:LEU:HD13	1:A:411:MET:HB2	2.00	0.44
1:A:81:ARG:HA	1:A:84:TYR:CE2	2.53	0.44
1:A:214:TYR:CZ	1:A:385:GLY:HA3	2.53	0.44
1:A:432:ALA:HB1	1:A:439:LYS:HG2	2.00	0.44

*Continued on next page...*



Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:103:ILE:O	1:A:516:TYR:OH	2.36	0.43
1:A:87:TYR:OH	1:A:376:ILE:O	2.26	0.43
1:A:500:ARG:NH2	1:A:597:GLU:OE2	2.51	0.43
1:A:221:LEU:HD13	1:A:466:ILE:CG2	2.48	0.43
1:A:425:GLU:OE1	1:A:442:ARG:NH2	2.49	0.43
2:B:87:PRO:O	2:B:90:THR:HG22	2.18	0.43
2:B:37:TYR:O	2:B:94:TYR:N	2.45	0.43
1:A:357:SER:O	1:A:361:ILE:HG23	2.20	0.42
1:A:365:LEU:HG	1:A:390:LEU:HD21	2.00	0.42
1:A:93:ALA:O	1:A:97:PRO:HD2	2.19	0.42
1:A:84:TYR:CE2	1:A:384:ALA:HA	2.54	0.42
1:A:265:ILE:O	1:A:269:LEU:HB2	2.20	0.42
1:A:532:VAL:HA	1:A:535:VAL:HG22	2.00	0.42
1:A:381:THR:CG2	1:A:386:LEU:HA	2.50	0.42
1:A:520:CYS:HA	1:A:524:VAL:HB	2.01	0.41
1:A:100:LEU:O	1:A:104:ILE:HG13	2.21	0.41
1:A:563:LEU:O	1:A:567:VAL:HG22	2.20	0.41
2:B:71:ARG:NH1	6:B:202:HOH:O	2.44	0.41
1:A:251:SER:HB3	1:A:421:MET:SD	2.61	0.41
1:A:269:LEU:HD23	1:A:269:LEU:HA	1.96	0.41
1:A:403:PHE:O	1:A:407:VAL:HG23	2.21	0.41
1:A:529:LEU:HA	1:A:532:VAL:HG22	2.03	0.41
1:A:553:TRP:HA	1:A:556:TRP:CE3	2.56	0.41
1:A:110:PHE:CE1	1:A:114:LEU:HD11	2.56	0.41
1:A:332:TYR:OH	6:A:801:HOH:O	2.20	0.41
1:A:86:CYS:SG	1:A:91:GLY:HA2	2.61	0.40
2:B:34:MET:HG3	2:B:78:VAL:HG21	2.03	0.40
1:A:121:ARG:NH2	1:A:333:ASN:O	2.48	0.40
1:A:274:LEU:HD11	1:A:357:SER:HA	2.02	0.40
1:A:211:ALA:HA	1:A:389:ILE:HG12	2.04	0.40
1:A:148:VAL:HG21	1:A:323:PHE:CE1	2.56	0.40
2:B:36:TRP:HD1	2:B:69:ILE:HD12	1.86	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM

entries.

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	542/571 (95%)	532 (98%)	10 (2%)	0	100	100
2	B	117/120 (98%)	114 (97%)	3 (3%)	0	100	100
All	All	659/691 (95%)	646 (98%)	13 (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 PDB entries followed by that with respect to all EM entries.

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	463/480 (96%)	448 (97%)	15 (3%)	34	60
2	B	98/99 (99%)	95 (97%)	3 (3%)	35	62
All	All	561/579 (97%)	543 (97%)	18 (3%)	37	60

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	100	LEU
1	A	101[A]	PHE
1	A	101[B]	PHE
1	A	190	LEU
1	A	205	TYR
1	A	253	TRP
1	A	269	LEU
1	A	298	ASP
1	A	350	ASN
1	A	373	LYS
1	A	399	SER
1	A	411	MET
1	A	471	LEU
1	A	481	ILE

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	610	GLN
2	B	19	ARG
2	B	45	ARG
2	B	72	ASP

Sometimes 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 oligosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 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	$\# Z  > 2$
3	LNR	A	701	-	12,12,12	4.93	6 (50%)	15,16,16	0.82	0
5	PTY	A	703	-	27,27,49	0.61	0	30,32,54	0.47	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
3	LNR	A	701	-	-	2/6/6/6	0/1/1/1
5	PTY	A	703	-	-	15/31/31/53	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	701	LNR	CAG-CAJ	9.90	1.52	1.38
3	A	701	LNR	CAF-CAK	8.41	1.52	1.39
3	A	701	LNR	CAE-CAI	7.23	1.52	1.39
3	A	701	LNR	CAI-CAJ	-5.03	1.32	1.40
3	A	701	LNR	CAG-CAK	-4.37	1.32	1.39
3	A	701	LNR	CAF-CAE	-4.13	1.31	1.38

There are no bond angle outliers.

There are no chirality outliers.

All (17) torsion outliers are listed below:

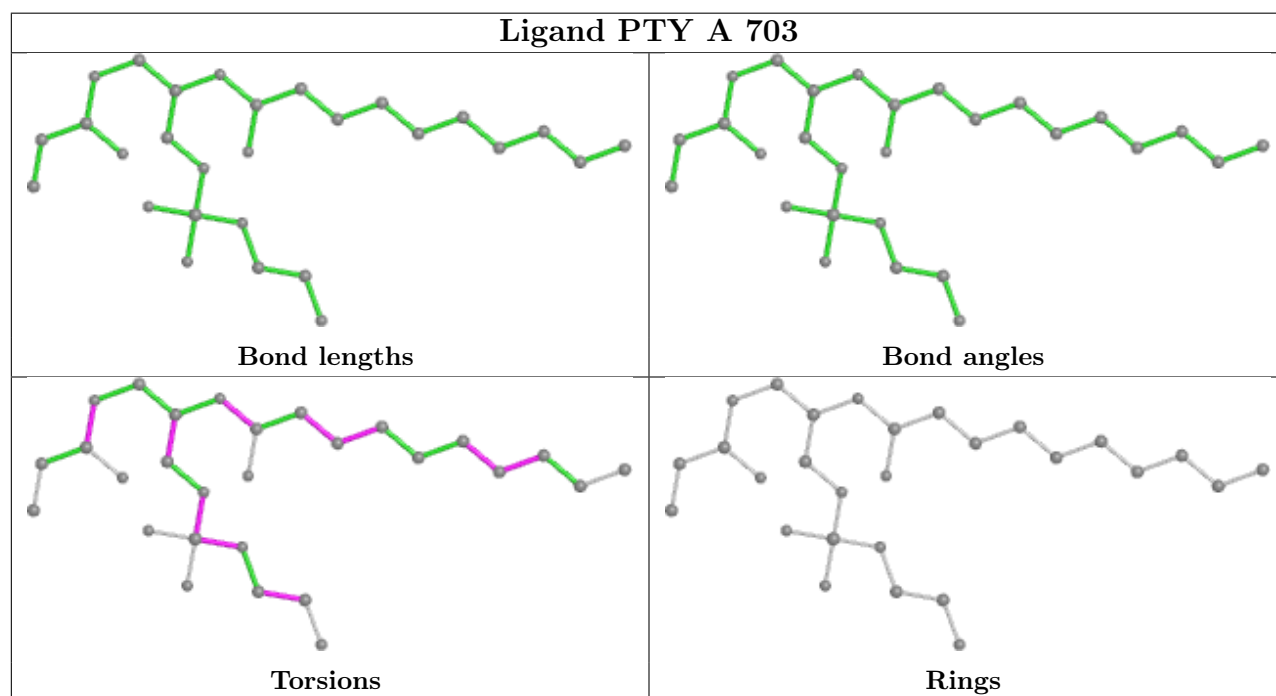
Mol	Chain	Res	Type	Atoms
3	A	701	LNR	NAA-CAH-CAL-OAD
5	A	703	PTY	C3-O11-P1-O12
5	A	703	PTY	C5-O14-P1-O13
5	A	703	PTY	O30-C30-O4-C1
5	A	703	PTY	C31-C30-O4-C1
5	A	703	PTY	C3-O11-P1-O14
5	A	703	PTY	C11-C8-O7-C6
5	A	703	PTY	C8-C11-C12-C13
5	A	703	PTY	O10-C8-O7-C6
5	A	703	PTY	C15-C16-C17-C18
3	A	701	LNR	NAA-CAH-CAL-CAK
5	A	703	PTY	N1-C2-C3-O11
5	A	703	PTY	C5-O14-P1-O11
5	A	703	PTY	C3-O11-P1-O13
5	A	703	PTY	C14-C15-C16-C17
5	A	703	PTY	C11-C12-C13-C14
5	A	703	PTY	O14-C5-C6-O7

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	703	PTY	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.