



wwPDB EM Validation Summary Report ⓘ

Oct 22, 2024 – 12:22 AM JST

PDB ID : 8JRU
EMDB ID : EMD-36606
Title : Cryo-EM structure of the glucagon receptor bound to beta-arrestin 1 in ligand-free state
Authors : Chen, K.; Zhang, C.; Lin, S.; Zhao, Q.; Wu, B.
Deposited on : 2023-06-17
Resolution : 3.50 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/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

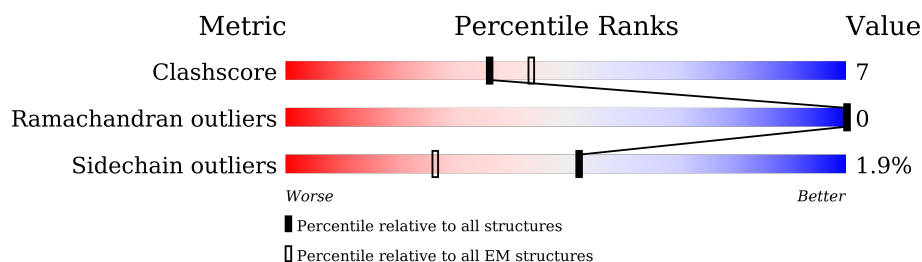
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.50 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 ≥ 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	R	478	
2	A	627	
2	H	627	
2	L	627	
3	B	126	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7120 atoms, of which 0 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 HA signal peptide,HPC4 purification tag,Glucagon receptor,C-terminal tail of Vasopressin V2 receptor.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	R	267	Total	C	N	O	P	S	0	0
			2008	1319	332	346	5	6		

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	-16	GLY	-	expression tag	UNP P03435
R	-15	SER	-	expression tag	UNP P03435
R	2	GLY	-	linker	UNP P03435
R	3	ALA	-	linker	UNP P03435
R	4	PRO	-	linker	UNP P03435
R	17	GLY	-	linker	UNP P04070
R	18	SER	-	linker	UNP P04070
R	19	GLY	-	linker	UNP P04070
R	20	SER	-	linker	UNP P04070
R	21	ALA	-	linker	UNP P04070
R	22	GLY	-	linker	UNP P04070
R	23	SER	-	linker	UNP P04070
R	24	ALA	-	linker	UNP P04070
R	25	GLY	-	linker	UNP P04070
R	26	SER	-	linker	UNP P04070

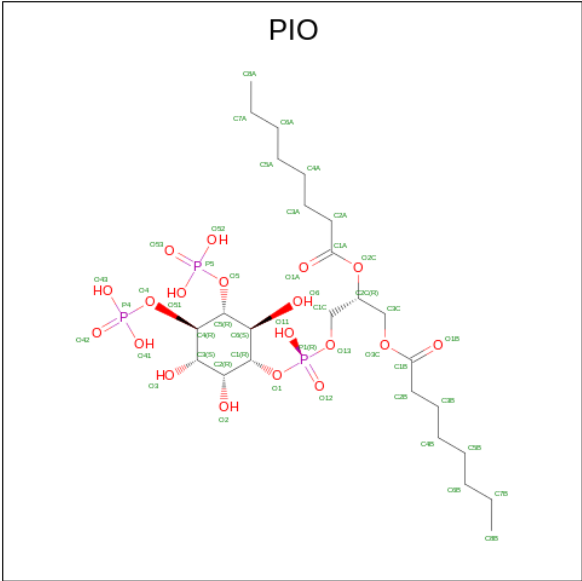
- Molecule 2 is a protein called Beta-arrestin 1 and single-chain fragment variable 30 (scFv30).

Mol	Chain	Residues	Atoms						AltConf	Trace
2	A	346	Total	C	N	O	S		0	0
			2576	1657	442	474	3			
2	H	117	Total	C	N	O	S		0	0
			891	569	150	170	2			
2	L	107	Total	C	N	O	S		0	0
			790	501	130	157	2			

- Molecule 3 is a protein called Nanobody 32.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	B	110	815	507	145	159	4	0	0

- Molecule 4 is [(2R)-2-octanoyloxy-3-[oxidanyl-[(1R,2R,3S,4R,5R,6S)-2,3,6-tris(oxidanyl)-4,5-diphosphonoxy-cyclohexyl]oxy-phosphoryl]oxy-propyl] octanoate (three-letter code: PIO) (formula: C₂₅H₄₉O₁₉P₃) (labeled as "Ligand of Interest" by depositor).

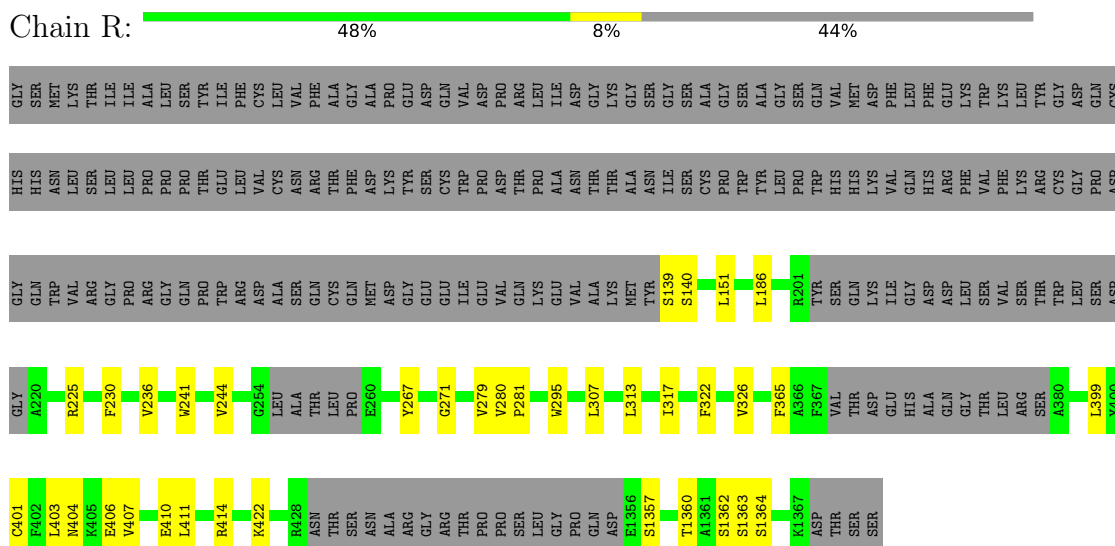


Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
4	A	1	40	18	19	3	0

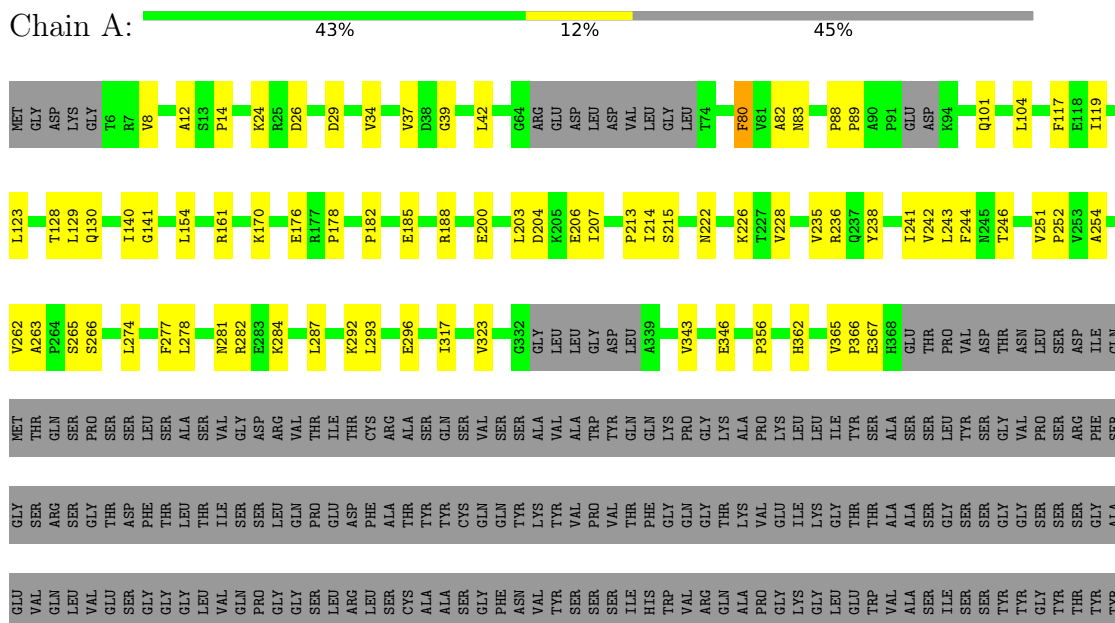
3 Residue-property plots

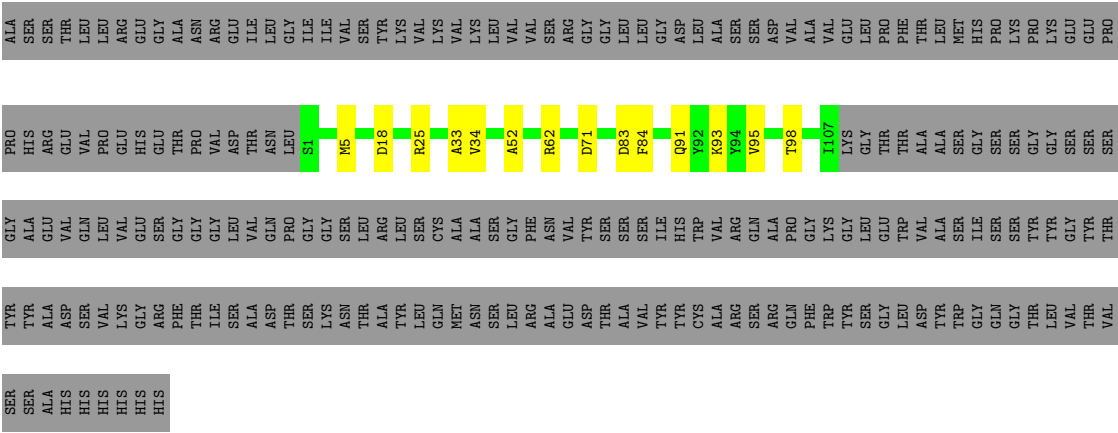
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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: HA signal peptide,HPC4 purification tag,Glucagon receptor,C-terminal tail of Vasopressin V2 receptor

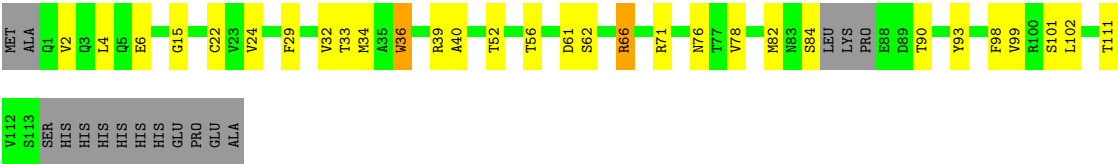


- Molecule 2: Beta-arrestin 1 and single-chain fragment variable 30 (scFv30)





● Molecule 3: Nanobody 32



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	250907	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 ($e^-/\text{\AA}^2$)	70	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k 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: PIO, TPO, SEP

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	R	0.24	0/2000	0.48	0/2726
2	A	0.24	0/2635	0.48	0/3606
2	H	0.25	0/915	0.49	0/1246
2	L	0.26	0/808	0.51	0/1103
3	B	0.27	0/829	0.59	0/1126
All	All	0.25	0/7187	0.50	0/9807

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	R	2008	0	1906	18	0
2	A	2576	0	2492	47	0
2	H	891	0	833	20	0
2	L	790	0	742	7	0
3	B	815	0	765	18	0
4	A	40	0	24	0	0
All	All	7120	0	6762	104	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.

The worst 5 of 104 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)
3:B:34:MET:HG3	3:B:78:VAL:HG11	1.63	0.78
1:R:241:TRP:HE3	1:R:271:GLY:HA3	1.58	0.67
2:A:37:VAL:HB	2:A:117:PHE:HB2	1.77	0.66
2:L:91:GLN:HE21	2:L:98:THR:H	1.41	0.66
1:R:406:GLU:N	1:R:406:GLU:OE2	2.30	0.64

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	R	252/478 (53%)	239 (95%)	13 (5%)	0	100	100
2	A	338/627 (54%)	317 (94%)	21 (6%)	0	100	100
2	H	115/627 (18%)	113 (98%)	2 (2%)	0	100	100
2	L	105/627 (17%)	98 (93%)	7 (7%)	0	100	100
3	B	106/126 (84%)	98 (92%)	8 (8%)	0	100	100
All	All	916/2485 (37%)	865 (94%)	51 (6%)	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	R	182/404 (45%)	180 (99%)	2 (1%)	70	83
2	A	264/538 (49%)	263 (100%)	1 (0%)	89	95
2	H	89/538 (16%)	84 (94%)	5 (6%)	17	45
2	L	82/538 (15%)	80 (98%)	2 (2%)	44	68
3	B	83/104 (80%)	80 (96%)	3 (4%)	30	59
All	All	700/2122 (33%)	687 (98%)	13 (2%)	52	73

5 of 13 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	H	93	ASP
2	L	18	ASP
3	B	82	MET
3	B	36	TRP
3	B	66	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
2	H	42	GLN
2	L	91	GLN
3	B	76	ASN
1	R	392	GLN
1	R	361	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

5 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
1	SEP	R	1357	1	8,9,10	1.56	1 (12%)	8,12,14	1.70	2 (25%)
1	SEP	R	1362	1	8,9,10	1.55	1 (12%)	8,12,14	1.56	2 (25%)
1	TPO	R	1360	1	8,10,11	1.59	1 (12%)	10,14,16	1.85	1 (10%)
1	SEP	R	1364	1	8,9,10	1.55	1 (12%)	8,12,14	1.53	2 (25%)
1	SEP	R	1363	1	8,9,10	1.55	1 (12%)	8,12,14	1.62	2 (25%)

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
1	SEP	R	1357	1	-	3/5/8/10	-
1	SEP	R	1362	1	-	1/5/8/10	-
1	TPO	R	1360	1	-	1/9/11/13	-
1	SEP	R	1364	1	-	1/5/8/10	-
1	SEP	R	1363	1	-	1/5/8/10	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	R	1357	SEP	P-O1P	3.40	1.61	1.50
1	R	1363	SEP	P-O1P	3.39	1.61	1.50
1	R	1364	SEP	P-O1P	3.38	1.61	1.50
1	R	1360	TPO	P-O1P	3.37	1.61	1.50
1	R	1362	SEP	P-O1P	3.36	1.61	1.50

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	R	1360	TPO	P-OG1-CB	-5.37	106.98	123.21
1	R	1357	SEP	OG-CB-CA	3.14	111.20	108.14
1	R	1357	SEP	P-OG-CB	-3.08	109.82	118.30
1	R	1362	SEP	P-OG-CB	-2.98	110.09	118.30
1	R	1363	SEP	P-OG-CB	-2.96	110.14	118.30

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	R	1357	SEP	CA-CB-OG-P
1	R	1357	SEP	CB-OG-P-O1P
1	R	1363	SEP	N-CA-CB-OG
1	R	1360	TPO	C-CA-CB-CG2
1	R	1364	SEP	N-CA-CB-OG

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand is 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	$\# Z > 2$
4	PIO	A	701	-	40,40,47	0.81	1 (2%)	54,58,65	1.45	6 (11%)

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
4	PIO	A	701	-	-	20/37/61/68	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	701	PIO	P4-O4	2.40	1.63	1.59

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	701	PIO	P1-O1-C1	6.58	143.34	119.41
4	A	701	PIO	O2C-C1A-C2A	4.15	120.44	111.50
4	A	701	PIO	C2C-O2C-C1A	3.95	127.52	117.79
4	A	701	PIO	O2C-C2C-C3C	3.09	119.57	108.40
4	A	701	PIO	C3A-C2A-C1A	2.42	122.41	113.62

There are no chirality outliers.

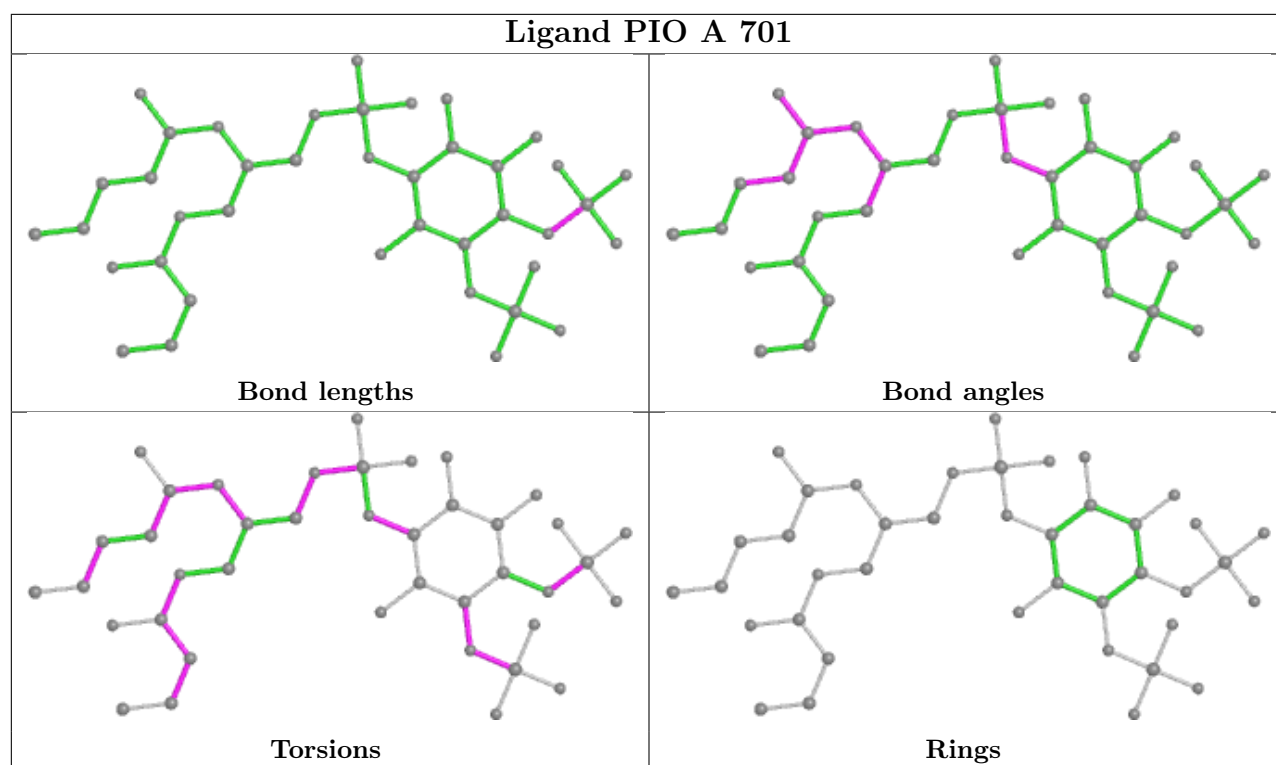
5 of 20 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	701	PIO	C2-C1-O1-P1
4	A	701	PIO	C1C-O13-P1-O1
4	A	701	PIO	C1C-O13-P1-O11
4	A	701	PIO	C1C-O13-P1-O12
4	A	701	PIO	C4-C5-O5-P5

There are no ring outliers.

No monomer is involved in short contacts.

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.