



## Full wwPDB EM Validation Report ⓘ

Dec 7, 2025 – 12:48 AM JST

PDB ID : 9JQY / pdb\_00009jqy  
EMDB ID : EMD-61743  
Title : Structural Insights into Selective Antagonism of TG6-129 and EP4  
Prostaglandin Receptor  
Authors : Wu, Y.L.; Zhang, H.; Xu, J.Y.; Wu, C.R.; Xu, E.H.  
Deposited on : 2024-09-28  
Resolution : 2.92 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>.

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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 : 4-5-2 with Phenix2.0  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
EM percentile statistics : **NOT EXECUTED**  
MapQ : **FAILED**  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.46

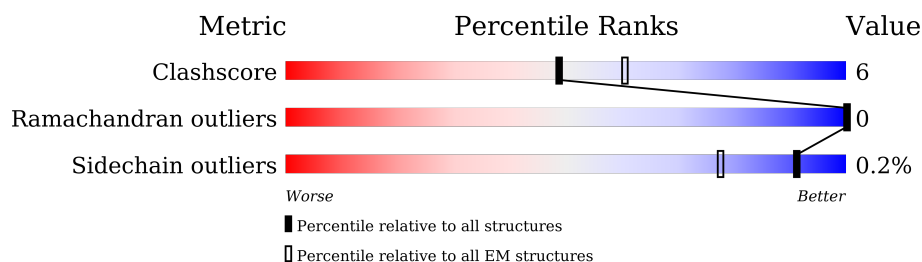
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.92 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	H	253	
2	L	255	
3	A	549	

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5350 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 Heavy chain of Fab fragment.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	H	204	Total	C	N	O	S	1	0
			1570	1009	251	304	6		

- Molecule 2 is a protein called Light chain of Fab fragment.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	L	197	Total	C	N	O	S	0	0
			1533	961	254	309	9		

- Molecule 3 is a protein called GFP-like fluorescent chromoprotein, Prostaglandin E2 receptor EP4 subtype.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	281	Total	C	N	O	S	0	0
			2209	1458	358	377	16		

There are 47 discrepancies between the modelled and reference sequences:

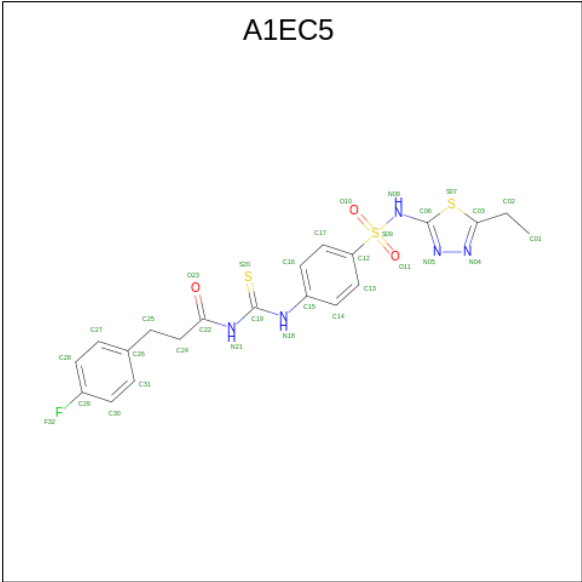
Chain	Residue	Modelled	Actual	Comment	Reference
A	0	ALA	THR	engineered mutation	UNP P35408
A	4	GLN	ASN	engineered mutation	UNP P35408
A	59	LEU	ALA	engineered mutation	UNP P35408
A	103	ARG	GLY	engineered mutation	UNP P35408
A	174	GLN	ASN	engineered mutation	UNP P35408
A	?	-	MET	deletion	UNP P35408
A	?	-	ARG	deletion	UNP P35408
A	?	-	ARG	deletion	UNP P35408
A	?	-	THR	deletion	UNP P35408
A	?	-	SER	deletion	UNP P35408
A	?	-	LEU	deletion	UNP P35408
A	?	-	GLY	deletion	UNP P35408
A	?	-	THR	deletion	UNP P35408
A	?	-	GLU	deletion	UNP P35408

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	GLN	deletion	UNP P35408
A	?	-	HIS	deletion	UNP P35408
A	?	-	HIS	deletion	UNP P35408
A	?	-	ALA	deletion	UNP P35408
A	?	-	ALA	deletion	UNP P35408
A	?	-	ALA	deletion	UNP P35408
A	?	-	ALA	deletion	UNP P35408
A	?	-	ALA	deletion	UNP P35408
A	?	-	SER	deletion	UNP P35408
A	?	-	VAL	deletion	UNP P35408
A	?	-	ALA	deletion	UNP P35408
A	?	-	SER	deletion	UNP P35408
A	?	-	ARG	deletion	UNP P35408
A	?	-	GLY	deletion	UNP P35408
A	?	-	HIS	deletion	UNP P35408
A	?	-	PRO	deletion	UNP P35408
A	?	-	ALA	deletion	UNP P35408
A	?	-	ALA	deletion	UNP P35408
A	?	-	SER	deletion	UNP P35408
A	?	-	PRO	deletion	UNP P35408
A	?	-	ALA	deletion	UNP P35408
A	?	-	LEU	deletion	UNP P35408
A	?	-	PRO	deletion	UNP P35408
A	?	-	ARG	deletion	UNP P35408
A	?	-	LEU	deletion	UNP P35408
A	?	-	SER	deletion	UNP P35408
A	?	-	ASP	deletion	UNP P35408
A	?	-	PHE	deletion	UNP P35408
A	?	-	ARG	deletion	UNP P35408
A	?	-	ARG	deletion	UNP P35408
A	?	-	ARG	deletion	UNP P35408
A	?	-	ARG	deletion	UNP P35408
A	?	-	SER	deletion	UNP P35408

- Molecule 4 is {N}-[[4-[(5-ethyl-1,3,4-thiadiazol-2-yl)sulfamoyl]phenyl]carbamoithiyl]-3-(4-fluorophenyl)propanamide (CCD ID: A1EC5) (formula: C<sub>20</sub>H<sub>20</sub>FN<sub>5</sub>O<sub>3</sub>S<sub>3</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						AltConf
			Total	C	F	N	O	S	
4	A	1	32	20	1	5	3	3	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	AltConf
5	A	6	Total O 6 6	0



K263	N264	P265	R271	S274	I278	R288	K289	T290	I296	GLU	LYS	ILE	LYS	CYS	LEU	PHE	CYS	ARG	ILE	GLY	GLY	SER	ARG	ARG	GLU	ARG	SER	GLY	GLN	HIS	CYS	SER	ASP	SER
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## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	97395	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOCONTINUUM (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: A1EC5

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	H	0.10	0/1614	0.26	0/2205
2	L	0.10	0/1567	0.28	0/2123
3	A	0.11	0/2261	0.26	0/3084
All	All	0.11	0/5442	0.27	0/7412

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	H	1570	0	1500	18	0
2	L	1533	0	1460	22	0
3	A	2209	0	2301	23	0
4	A	32	0	0	4	0
5	A	6	0	0	1	0
All	All	5350	0	5261	59	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 6.

All (59) 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:A:246:ARG:HD2	3:A:265:PRO:HB2	1.71	0.73
3:A:50:THR:HG23	3:A:133:ALA:HB2	1.70	0.73
1:H:110:SER:HA	1:H:136:VAL:O	1.90	0.71
1:H:53:ILE:HD11	1:H:115:CYS:HB2	1.73	0.69
2:L:53:ARG:HH21	2:L:74:ASN:HD22	1.43	0.66
3:A:274:SER:OG	4:A:401:A1EC5:C01	2.45	0.65
2:L:177:ARG:HH12	2:L:179:ASN:HB3	1.64	0.62
3:A:79:LYS:HE2	3:A:81:GLN:HE21	1.66	0.60
1:H:102:LEU:HB3	1:H:105:LEU:HD21	1.86	0.58
2:L:29:SER:OG	2:L:44:THR:OG1	2.22	0.57
1:H:54:TYR:HB3	1:H:66:TRP:HZ3	1.70	0.56
3:A:207:LEU:HD11	3:A:226:VAL:HG21	1.88	0.56
2:L:130:ARG:HD3	2:L:193:SER:HB2	1.86	0.55
3:A:114:ARG:NH1	3:A:222:GLU:OE1	2.40	0.55
2:L:113:TYR:HD2	3:A:259:ARG:HH12	1.55	0.54
3:A:58:LEU:HB2	3:A:106:ILE:HG21	1.90	0.54
3:A:151:PRO:HA	3:A:156:GLY:H	1.73	0.53
1:H:221:THR:HG22	1:H:236:LYS:HG2	1.90	0.52
2:L:53:ARG:HH12	2:L:72:ARG:HE	1.56	0.52
3:A:288:ARG:NH1	3:A:290:THR:OG1	2.44	0.51
3:A:193:ILE:HG23	3:A:237:LEU:HD22	1.93	0.51
2:L:187:ASP:OD1	2:L:188:GLN:N	2.45	0.50
2:L:220:HIS:CD2	2:L:221:LYS:H	2.29	0.50
3:A:21:PRO:HG3	4:A:401:A1EC5:O11	2.14	0.48
1:H:33:PRO:HG2	1:H:140:ALA:HB2	1.94	0.48
3:A:18:VAL:HG22	3:A:77:TYR:HB3	1.96	0.47
3:A:69:VAL:HG11	4:A:401:A1EC5:C01	2.45	0.46
2:L:155:VAL:HG22	2:L:200:THR:HG22	1.97	0.46
2:L:70:ILE:HG12	2:L:76:MET:HG2	1.97	0.46
2:L:169:LYS:HD3	2:L:171:LYS:HE2	1.98	0.46
2:L:207:GLU:OE2	2:L:211:HIS:NE2	2.44	0.45
2:L:87:SER:OG	2:L:94:SER:OG	2.35	0.45
1:H:194:PRO:HD3	2:L:186:THR:HG22	1.99	0.45
1:H:79:TYR:O	1:H:84:ARG:NH2	2.50	0.45
1:H:80:ASN:OD1	1:H:81:GLN:N	2.50	0.45
3:A:44:LYS:HG2	3:A:52:TYR:HD2	1.81	0.45
1:H:29:GLU:HB2	1:H:136:VAL:HG22	1.98	0.44
1:H:196:VAL:HG11	2:L:182:LEU:HB3	1.98	0.44
2:L:167:ASN:HB3	2:L:219:THR:OG1	2.18	0.44
3:A:69:VAL:CG1	4:A:401:A1EC5:C01	2.96	0.44
3:A:260:GLU:HB2	3:A:263:LYS:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:71:ASP:OD2	1:H:120:TYR:OH	2.31	0.43
3:A:271:ARG:NH1	5:A:501:HOH:O	2.52	0.43
1:H:73:TYR:OH	3:A:164:ASP:OD1	2.29	0.42
2:L:142:PRO:HD3	2:L:154:VAL:HG22	2.01	0.42
2:L:189:ASP:OD1	2:L:189:ASP:N	2.52	0.42
2:L:28:GLN:HE21	2:L:43:ILE:HG21	1.84	0.42
3:A:24:MET:HB3	3:A:278:ILE:HD13	2.01	0.42
2:L:130:ARG:HG2	2:L:131:ALA:H	1.83	0.41
2:L:188:GLN:HE21	2:L:193:SER:HB3	1.84	0.41
2:L:167:ASN:HB3	2:L:219:THR:HG1	1.85	0.41
1:H:115:CYS:O	1:H:131:GLY:N	2.54	0.41
3:A:25:PHE:HE1	3:A:67:LEU:HD23	1.86	0.41
1:H:21:ILE:HA	1:H:44:SER:O	2.21	0.41
1:H:36:SER:HA	1:H:102:LEU:O	2.21	0.41
1:H:173:PHE:HB3	1:H:174:PRO:HD3	2.03	0.41
3:A:21:PRO:HG2	3:A:77:TYR:HD2	1.86	0.40
3:A:68:LEU:HD12	3:A:99:PHE:CE2	2.56	0.40
1:H:43:ALA:HB1	1:H:46:PHE:CD1	2.57	0.40

There are no symmetry-related clashes.

## 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 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	H	195/253 (77%)	192 (98%)	3 (2%)	0	100	100
2	L	193/255 (76%)	189 (98%)	4 (2%)	0	100	100
3	A	279/549 (51%)	277 (99%)	2 (1%)	0	100	100
All	All	667/1057 (63%)	658 (99%)	9 (1%)	0	100	100

There are no Ramachandran outliers to report.

### 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 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	H	174/219 (80%)	174 (100%)	0	100	100
2	L	174/230 (76%)	174 (100%)	0	100	100
3	A	246/471 (52%)	245 (100%)	1 (0%)	89	96
All	All	594/920 (65%)	593 (100%)	1 (0%)	91	98

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	171	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	74	ASN
1	H	81	GLN
2	L	59	GLN
2	L	60	GLN
2	L	74	ASN
2	L	91	GLN
2	L	183	ASN
3	A	46	GLN
3	A	81	GLN
3	A	268	GLN
3	A	276	ASN

### 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](#)

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	A1EC5	A	401	-	31,34,34	2.86	14 (45%)	38,47,47	2.80	5 (13%)

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	A1EC5	A	401	-	-	6/22/26/26	0/3/3/3

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	401	A1EC5	C02-C03	6.03	1.53	1.49
4	A	401	A1EC5	C19-N18	5.93	1.45	1.35
4	A	401	A1EC5	N05-N04	5.79	1.49	1.37
4	A	401	A1EC5	S09-N08	4.84	1.71	1.63
4	A	401	A1EC5	C22-N21	4.80	1.46	1.37
4	A	401	A1EC5	C25-C24	-4.21	1.31	1.52
4	A	401	A1EC5	C19-N21	4.08	1.46	1.39
4	A	401	A1EC5	C12-S09	3.29	1.81	1.76
4	A	401	A1EC5	C06-N08	3.25	1.45	1.40
4	A	401	A1EC5	C03-S07	-3.16	1.63	1.73
4	A	401	A1EC5	C19-S20	-3.15	1.60	1.68
4	A	401	A1EC5	O10-S09	2.91	1.46	1.43
4	A	401	A1EC5	O11-S09	2.33	1.46	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	401	A1EC5	O23-C22	-2.21	1.18	1.23

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	401	A1EC5	O11-S09-O10	-14.84	101.31	119.55
4	A	401	A1EC5	C12-S09-N08	3.79	111.61	106.83
4	A	401	A1EC5	C24-C25-C26	2.94	123.43	112.70
4	A	401	A1EC5	O10-S09-C12	2.65	111.23	107.97
4	A	401	A1EC5	C30-C29-C28	-2.08	120.06	122.83

There are no chirality outliers.

All (6) torsion outliers are listed below:

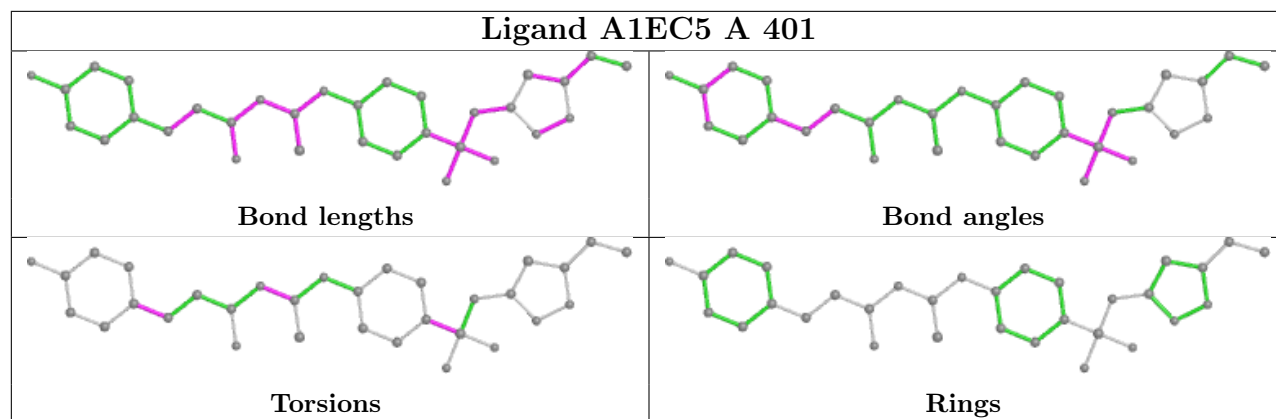
Mol	Chain	Res	Type	Atoms
4	A	401	A1EC5	C13-C12-S09-O11
4	A	401	A1EC5	C24-C25-C26-C31
4	A	401	A1EC5	C17-C12-S09-O11
4	A	401	A1EC5	C24-C25-C26-C27
4	A	401	A1EC5	S20-C19-N21-C22
4	A	401	A1EC5	N18-C19-N21-C22

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	401	A1EC5	4	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.