



## wwPDB EM Validation Summary Report ⓘ

Oct 7, 2024 – 02:22 PM JST

PDB ID : 8JIU  
EMDB ID : EMD-36328  
Title : Cryo-EM structure of the GLP-1R/GCGR dual agonist SAR425899-bound human GCGR-Gs complex  
Authors : Yang, L.; Zhou, Q.T.; Dai, A.T.; Zhao, F.H.; Chang, R.L.; Ying, T.L.; Wu, B.L.; Yang, D.H.; Wang, M.W.; Cong, Z.T.  
Deposited on : 2023-05-27  
Resolution : 2.76 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](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

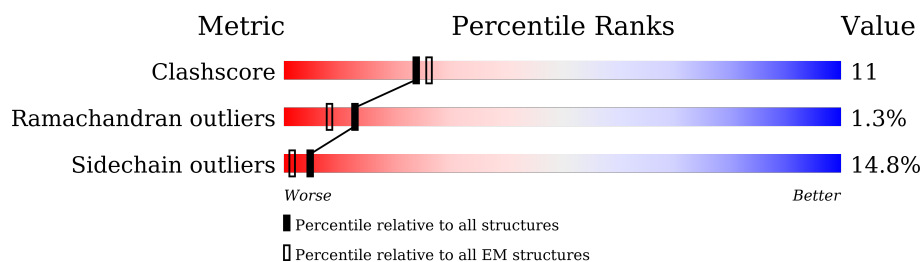
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.76 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	394	50% 8% . 41%
2	P	29	59% 31% 10%
3	B	345	74% 22% . .
4	C	70	56% 20% . 20%
5	N	140	64% 26% . 9%
6	R	405	59% 30% 8% .

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 9075 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 Guanine nucleotide-binding protein G(s) subunit alpha isoforms short.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	231	Total	C	N	O	S	0	0
			1875	1186	339	343	7		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	54	ASN	SER	conflict	UNP P63092
A	226	ALA	GLY	conflict	UNP P63092
A	268	ALA	GLU	conflict	UNP P63092
A	271	LYS	ASN	conflict	UNP P63092
A	274	ASP	LYS	conflict	UNP P63092
A	280	LYS	ARG	variant	UNP P63092
A	284	ASP	THR	conflict	UNP P63092
A	285	THR	ILE	conflict	UNP P63092

- Molecule 2 is a protein called SAR425899.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	P	29	Total	C	N	O	0	0
			224	140	38	46		

- Molecule 3 is a protein called Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B	339	Total	C	N	O	S	0	0
			2548	1574	454	499	21		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-4	MET	-	initiating methionine	UNP P54311

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
B	-3	GLY	-	expression tag	UNP P54311
B	-2	SER	-	expression tag	UNP P54311
B	-1	LEU	-	expression tag	UNP P54311
B	0	LEU	-	expression tag	UNP P54311
B	1	GLN	-	expression tag	UNP P54311

- Molecule 4 is a protein called Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	C	56	Total	C	N	O	S	0	0
			420	263	73	81	3		

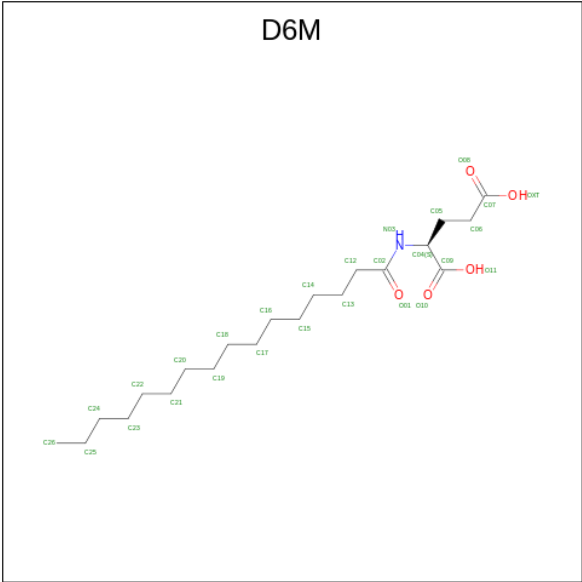
- Molecule 5 is a protein called Nanobody 35.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	N	128	Total	C	N	O	S	0	0
			964	601	169	188	6		

- Molecule 6 is a protein called Glucagon receptor.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	R	395	Total	C	N	O	S	0	0
			3018	1982	514	502	20		

- Molecule 7 is N-hexadecanoyl-L-glutamic acid (three-letter code: D6M) (formula: C<sub>21</sub>H<sub>39</sub>NO<sub>5</sub>).

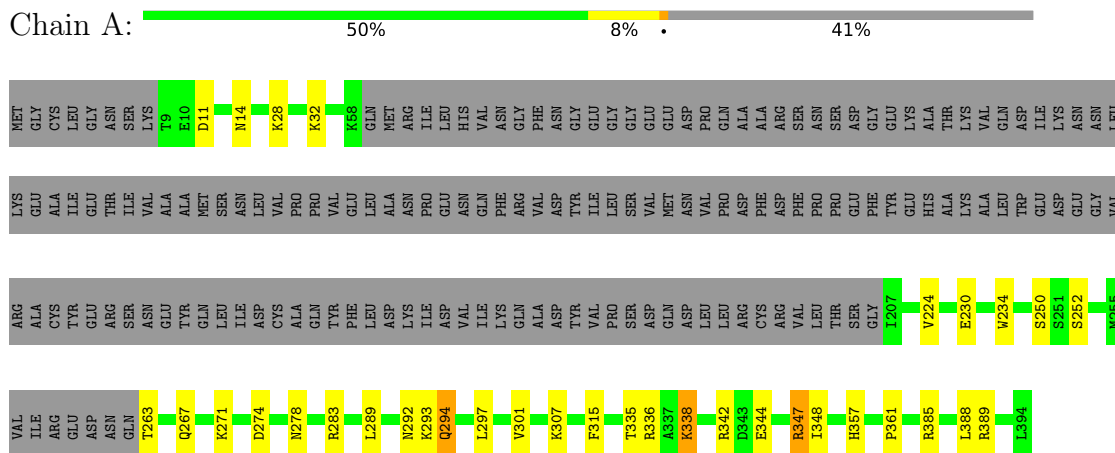


Mol	Chain	Residues	Atoms				AltConf
7	P	1	Total	C	N	O	0
			26	21	1	4	

### 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. 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.

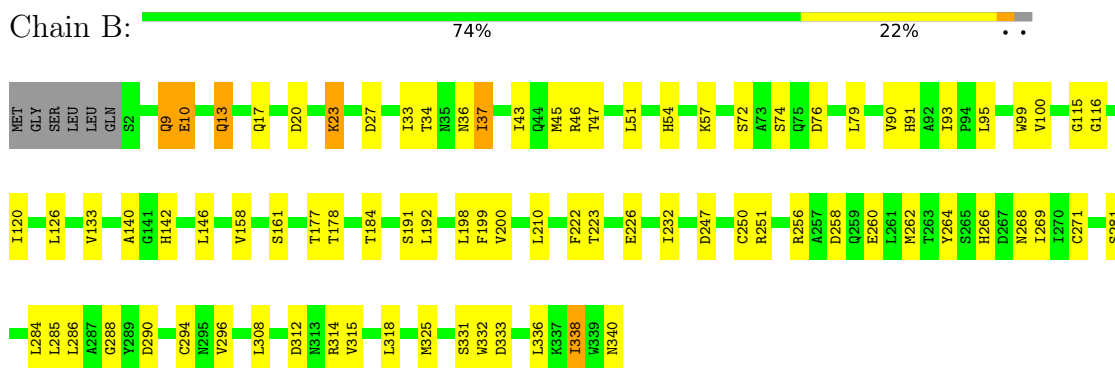
- Molecule 1: Guanine nucleotide-binding protein G(s) subunit alpha isoforms short



- Molecule 2: SAR425899

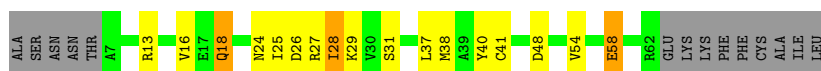


- Molecule 3: Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1



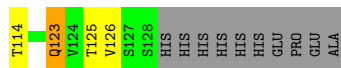
- Molecule 4: Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2





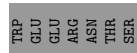
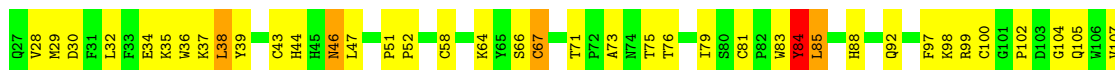
• Molecule 5: Nanobody 35

Chain N: 64% 26% 9%



• Molecule 6: Glucagon receptor

Chain R: 59% 30% 8%



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	828639	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	80	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor



## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: DSN, D6M

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	0.29	0/1911	0.43	0/2577
2	P	0.52	0/221	0.71	1/294 (0.3%)
3	B	0.32	0/2595	0.51	0/3525
4	C	0.42	0/426	0.59	0/576
5	N	0.38	0/984	0.58	0/1333
6	R	0.46	0/3103	0.63	0/4236
All	All	0.38	0/9240	0.56	1/12541 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	14	LYS	CD-CE-NZ	8.56	131.39	111.70

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

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	1875	0	1822	21	0
2	P	224	0	206	4	0
3	B	2548	0	2408	41	0
4	C	420	0	421	6	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	N	964	0	925	19	0
6	R	3018	0	2888	106	0
7	P	26	0	37	0	0
All	All	9075	0	8707	191	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 11.

The worst 5 of 191 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)
6:R:190:SER:OG	6:R:231:MET:HA	1.68	0.94
1:A:278:ASN:HD22	5:N:105:ARG:HE	1.22	0.88
6:R:156:LEU:HD11	6:R:184:PHE:HB3	1.54	0.88
6:R:151:LEU:O	6:R:151:LEU:HD12	1.80	0.80
6:R:153:LEU:HD12	6:R:153:LEU:O	1.84	0.78

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	225/394 (57%)	222 (99%)	3 (1%)	0	100	100
2	P	26/29 (90%)	25 (96%)	0	1 (4%)	2	3
3	B	337/345 (98%)	320 (95%)	17 (5%)	0	100	100
4	C	54/70 (77%)	46 (85%)	8 (15%)	0	100	100
5	N	126/140 (90%)	121 (96%)	4 (3%)	1 (1%)	16	29
6	R	393/405 (97%)	338 (86%)	42 (11%)	13 (3%)	3	4
All	All	1161/1383 (84%)	1072 (92%)	74 (6%)	15 (1%)	13	17

5 of 15 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	R	51	PRO
6	R	52	PRO
6	R	363	VAL
6	R	272	TRP
6	R	293	GLN

### 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	A	196/349 (56%)	189 (96%)	7 (4%)	30	51
2	P	22/23 (96%)	14 (64%)	8 (36%)	0	0
3	B	268/287 (93%)	244 (91%)	24 (9%)	8	14
4	C	43/57 (75%)	29 (67%)	14 (33%)	0	0
5	N	103/116 (89%)	95 (92%)	8 (8%)	10	19
6	R	296/353 (84%)	220 (74%)	76 (26%)	0	0
All	All	928/1185 (78%)	791 (85%)	137 (15%)	5	3

5 of 137 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	R	334	ARG
6	R	344	LYS
6	R	386	LEU
4	C	38	MET
4	C	37	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
6	R	131	GLN
6	R	291	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
6	R	392	GLN
6	R	372	HIS
6	R	46	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

1 non-standard protein/DNA/RNA residue 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	$\# Z  > 2$
2	DSN	P	2	2	4,5,6	0.59	0	0,5,7	-	-

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
2	DSN	P	2	2	-	2/2/4/6	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	P	2	DSN	N-CA-CB-OG
2	P	2	DSN	C-CA-CB-OG

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	P	2	DSN	2	0

## 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	$\# Z  > 2$
7	D6M	P	101	2	25,25,26	0.89	1 (4%)	27,27,29	1.23	1 (3%)

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
7	D6M	P	101	2	-	6/26/27/28	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	P	101	D6M	O08-C07	3.11	1.37	1.19

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	P	101	D6M	O08-C07-C06	-5.06	93.65	126.89

There are no chirality outliers.

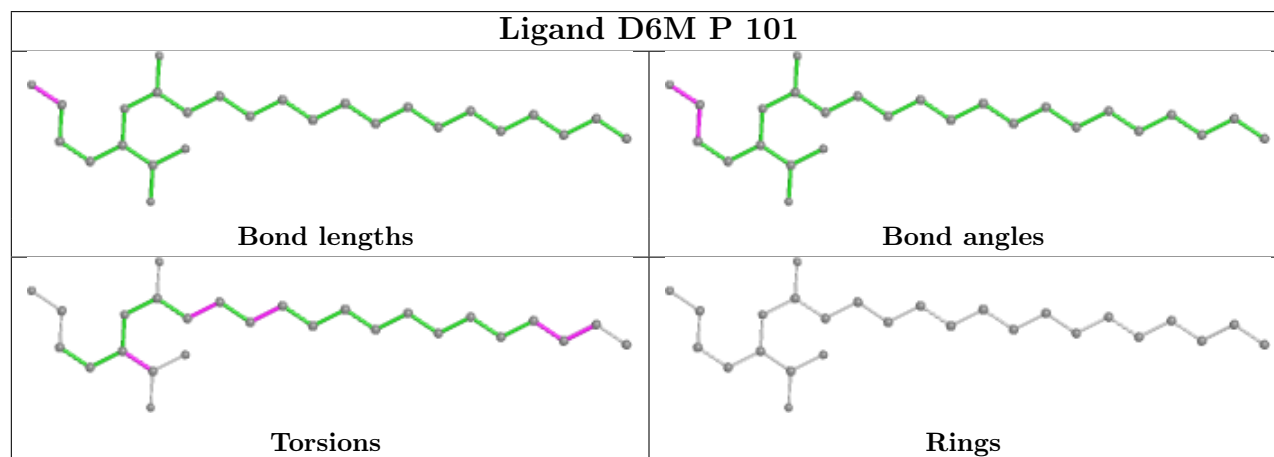
5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	P	101	D6M	C02-C12-C13-C14
7	P	101	D6M	C22-C23-C24-C25
7	P	101	D6M	C13-C14-C15-C16
7	P	101	D6M	N03-C04-C09-O11
7	P	101	D6M	N03-C04-C09-O10

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 ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.