



## wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Oct 29, 2019 – 02:47 PM EDT

PDB ID : 6J5U  
EMDB ID: : EMD-0681  
Title : Ligand-triggered allosteric ADP release primes a plant NLR complex  
Authors : Wang, J.Z.; Wang, J.; Meijuan, H.; Wang, H.W.; Zhou, J.M.; Chai, J.J.  
Deposited on : 2019-01-12  
Resolution : 3.90 Å(reported)  
Based on PDB ID : 3TL8

This is a wwPDB/EMDataBank EM Map/Model Validation Summary Report  
for a publicly released PDB/EMDB 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.

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MolProbity : 4.02b-467  
Mogul : 1.8.0 (224370), CSD as540be (2019)  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.4

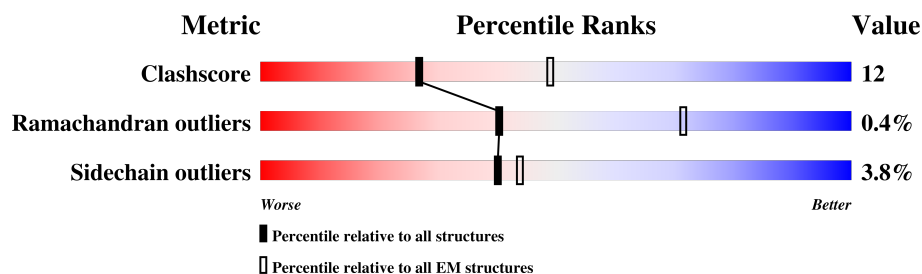
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.90 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	136327	1886
Ramachandran outliers	132723	1663
Sidechain outliers	132532	1531

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	852	
2	C	426	
3	B	351	

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 9288 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 Disease resistance RPP13-like protein 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	663	5266	3320	900	1010	36	0	0

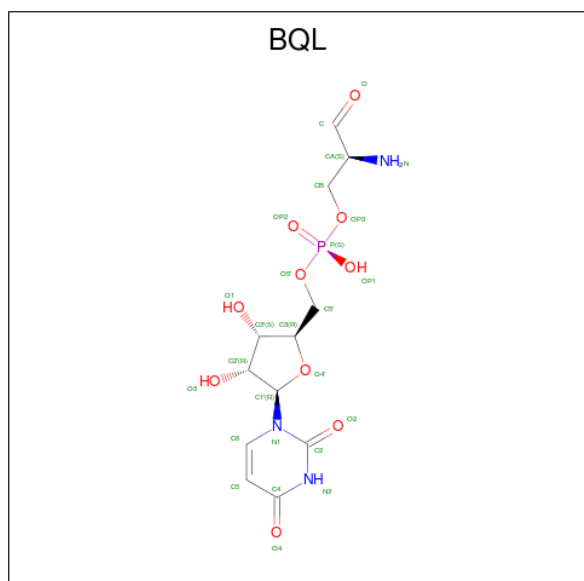
- Molecule 2 is a protein called Probable serine/threonine-protein kinase PBL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	C	172	1340	864	232	238	6	0	0

- Molecule 3 is a protein called Protein kinase superfamily protein.

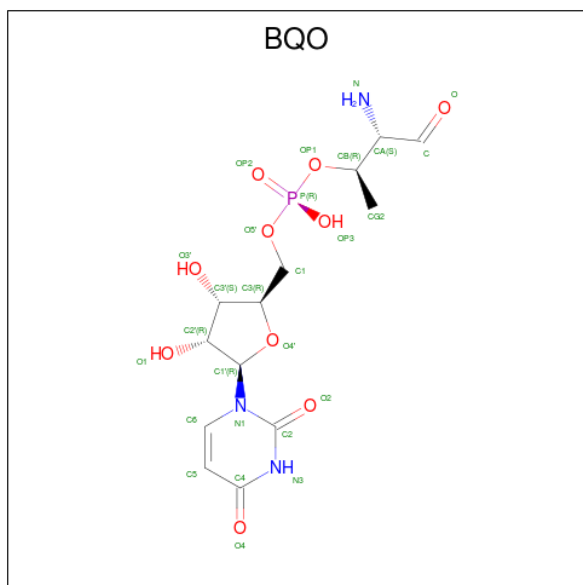
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	B	327	2629	1686	447	479	17	0	0

- Molecule 4 is [(2 {S})-2-azanyl-3-oxidanylidene-propyl] [(2 {R},3 {S},4 {R},5 {R})-5-[2,4-bis(oxidanylidene)pyrimidin-1-yl]-3,4-bis(oxidanyl)oxolan-2-yl]methyl hydrogen phosphate (three-letter code: BQL) (formula: C<sub>12</sub>H<sub>18</sub>N<sub>3</sub>O<sub>10</sub>P).



Mol	Chain	Residues	Atoms					AltConf
4	C	1	Total	C	N	O	P	0
			26	12	3	10	1	

- Molecule 5 is [(2 {R},3 {S})-3-azanyl-4-oxidanylidene-butan-2-yl] [(2 {R},3 {S},4 {R},5 {R})-5-[2,4-bis(oxidanylidene)pyrimidin-1-yl]-3,4-bis(oxidanyl)oxolan-2-yl]methyl hydrogen phosphate (three-letter code: BQO) (formula: C<sub>13</sub>H<sub>20</sub>N<sub>3</sub>O<sub>10</sub>P).



Mol	Chain	Residues	Atoms					AltConf
5	C	1	Total	C	N	O	P	0
			27	13	3	10	1	





## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	404311	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 ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	900	Depositor
Magnification	105000	Depositor
Image detector	GATAN K2 SUMMIT (4k 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: BQO, BQL

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	$\# Z  > 2$	RMSZ	$\# Z  > 2$
1	A	0.39	0/5365	0.75	7/7256 (0.1%)
2	C	0.33	0/1365	0.62	0/1841
3	B	0.44	0/2683	0.75	3/3621 (0.1%)
All	All	0.40	0/9413	0.73	10/12718 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	4
2	C	0	1
3	B	0	1
All	All	0	6

There are no bond length outliers.

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	663	LEU	CA-CB-CG	6.45	130.13	115.30
1	A	776	LEU	CA-CB-CG	6.03	129.16	115.30
3	B	276	LEU	CA-CB-CG	5.77	128.56	115.30
3	B	318	LEU	CA-CB-CG	5.71	128.44	115.30
1	A	418	CYS	CA-CB-SG	5.58	124.05	114.00

There are no chirality outliers.

5 of 6 planarity outliers are listed below:



Mol	Chain	Res	Type	Group
1	A	426	PRO	Peptide
1	A	531	LYS	Peptide
1	A	561	LEU	Peptide
1	A	649	CYS	Peptide
2	C	266	GLU	Peptide

## 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	5266	0	5258	141	0
2	C	1340	0	1365	29	0
3	B	2629	0	2654	53	0
4	C	26	0	0	0	0
5	C	27	0	0	0	0
All	All	9288	0	9277	220	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 12.

The worst 5 of 220 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:395:SER:O	1:A:399:ASN:CG	1.95	1.04
2:C:182:PHE:O	2:C:184:ARG:N	1.94	0.99
1:A:395:SER:C	1:A:399:ASN:OD1	2.01	0.98
1:A:498:ILE:O	1:A:502:ASP:HB2	1.75	0.85
1:A:358:LEU:HD21	1:A:400:VAL:HG11	1.60	0.82

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	657/852 (77%)	553 (84%)	103 (16%)	1 (0%)	49	83
2	C	162/426 (38%)	137 (85%)	23 (14%)	2 (1%)	14	55
3	B	323/351 (92%)	284 (88%)	38 (12%)	1 (0%)	43	79
All	All	1142/1629 (70%)	974 (85%)	164 (14%)	4 (0%)	40	74

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	183	ARG
1	A	403	SER
2	C	173	PRO
3	B	236	ASP

### 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	603/772 (78%)	583 (97%)	20 (3%)	41	70
2	C	139/355 (39%)	131 (94%)	8 (6%)	22	57
3	B	293/314 (93%)	282 (96%)	11 (4%)	36	66
All	All	1035/1441 (72%)	996 (96%)	39 (4%)	40	66

5 of 39 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	731	LYS
2	C	184	ARG
3	B	222	ARG
1	A	763	LEU
1	A	765	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	625	GLN
1	A	643	ASN
3	B	99	HIS
1	A	530	HIS
1	A	611	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](#)

There are no non-standard protein/DNA/RNA residues in this entry.

### 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

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

2 ligands 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	$\# Z  > 2$
4	BQL	C	501	2,5	22,27,27	0.84	0	22,39,39	1.17	4 (18%)
5	BQO	C	502	2,4	22,28,28	1.71	5 (22%)	23,41,41	1.55	4 (17%)

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	BQL	C	501	2,5	-	6/11/34/34	0/2/2/2
5	BQO	C	502	2,4	-	6/15/37/37	0/2/2/2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	502	BQO	O4'-C1'	4.85	1.48	1.41
5	C	502	BQO	C3'-C2'	-2.36	1.47	1.53
5	C	502	BQO	O4-C4	-2.34	1.18	1.24
5	C	502	BQO	C6-N1	-2.27	1.32	1.35
5	C	502	BQO	P-OP3	2.03	1.65	1.55

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	502	BQO	C3-O4'-C1'	-4.96	104.65	109.83
5	C	502	BQO	O-C-CA	-3.21	117.77	125.11
4	C	501	BQL	OP3-CB-CA	2.67	110.75	108.14
4	C	501	BQL	O4'-C1'-N1	2.35	112.64	108.06
4	C	501	BQL	C2'-C3'-C3	2.32	107.04	102.60

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

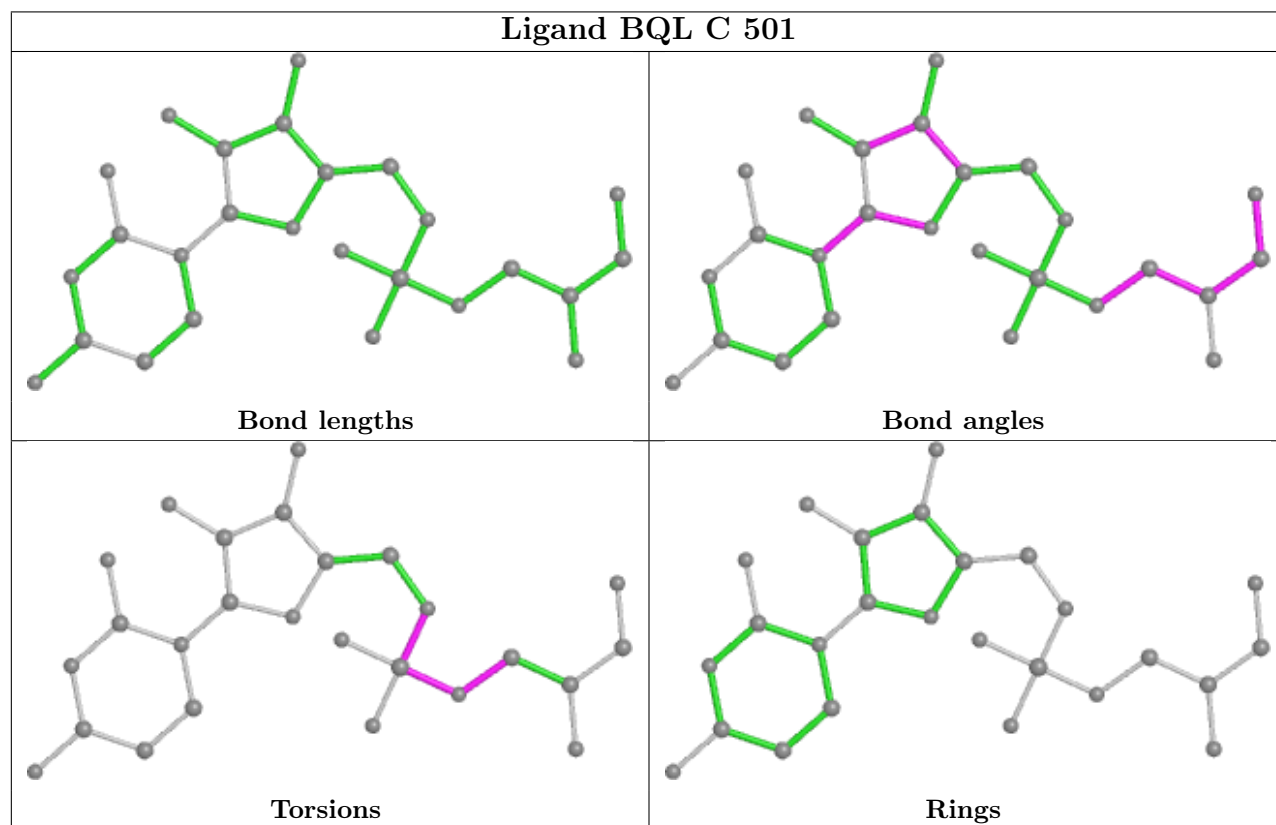
Mol	Chain	Res	Type	Atoms
5	C	502	BQO	O-C-CA-CB
5	C	502	BQO	N-CA-CB-OP1
5	C	502	BQO	C-CA-CB-CG2
4	C	501	BQL	CA-CB-OP3-P
4	C	501	BQL	C5'-O5'-P-OP2

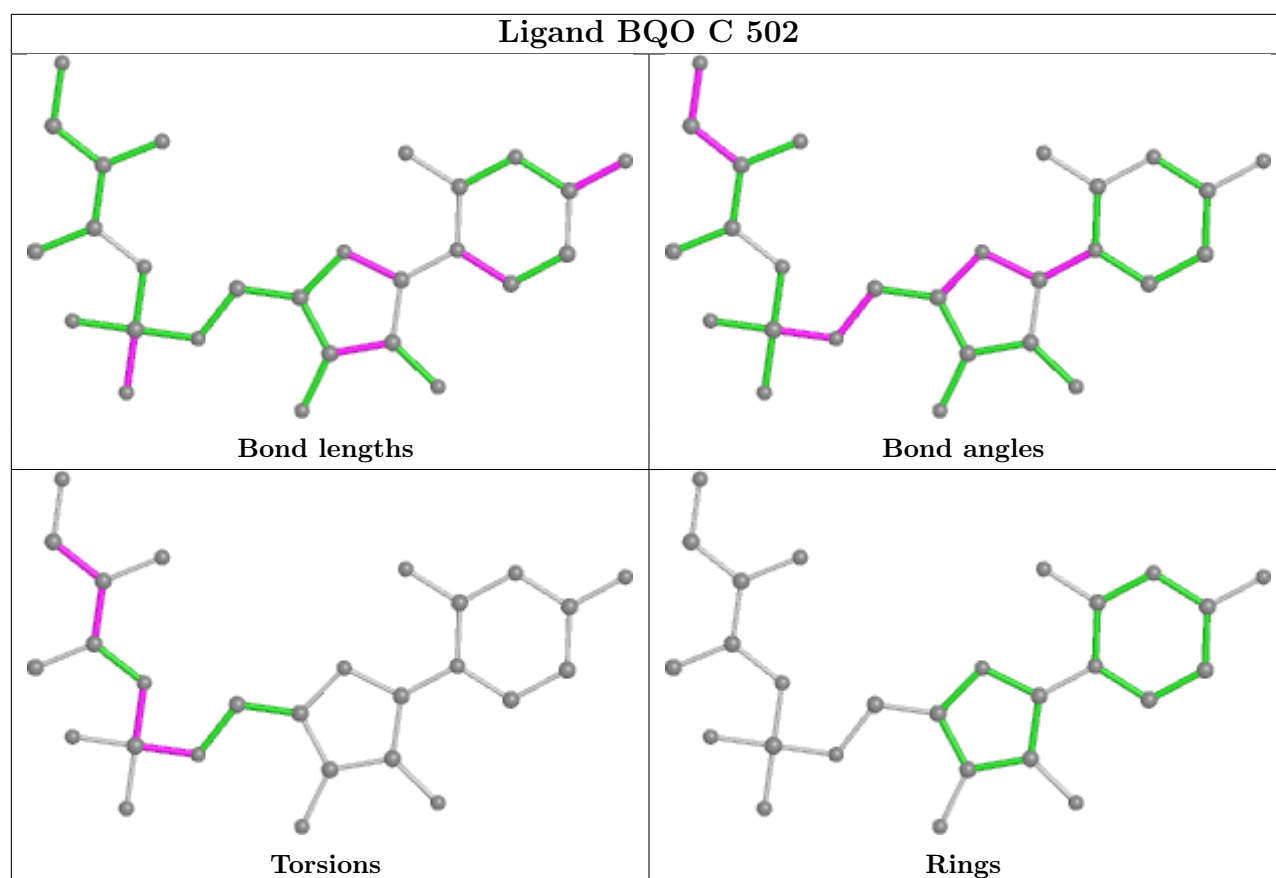
There are no ring outliers.

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.