



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 01:52 PM BST

PDB ID : 3JBG
EMDB ID: : EMD-6435
Title : Complex of poliovirus with VHH PVSS21E
Authors : Strauss, M.; Schotte, L.; Thys, B.; Filman, D.J.; Hogle, J.M.
Deposited on : 2015-08-26
Resolution : 3.80 Å(reported)
Based on PDB ID : 3QXU

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : trunk27241

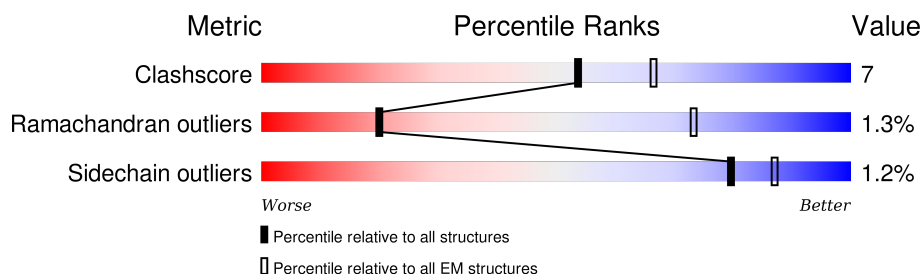
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.80 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	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

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 ≥ 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	1	302	80% 12% • 6%
2	2	272	91% 7% •
3	3	237	85% 13% ••
4	4	69	84% 13% ••
5	7	126	74% 21% ••

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	PLM	1	901	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 7599 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 Capsid protein VP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	283	Total	C	N	O	S	0	0
			2221	1416	378	422	5		

- Molecule 2 is a protein called Capsid protein VP2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	267	Total	C	N	O	S	0	0
			2075	1312	357	392	14		

- Molecule 3 is a protein called Capsid protein VP3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	3	235	Total	C	N	O	S	0	0
			1834	1169	299	349	17		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
3	123	SER	PHE	CONFLICT	UNP P03300

- Molecule 4 is a protein called Capsid protein VP4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	4	69	Total	C	N	O	S	0	0
			534	333	91	109	1		

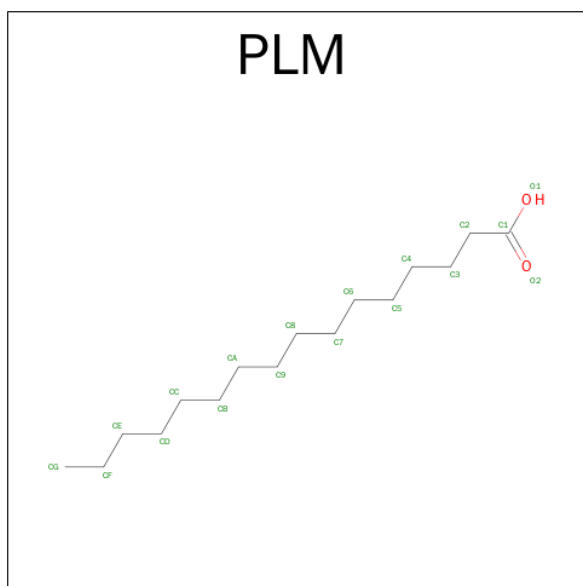
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
4	1	MYR	-	MYRISTOYLATION	UNP P03300

- Molecule 5 is a protein called nanobody VHH PVSS21E.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	7	121	Total	C	N	O	S	0	0
			921	570	166	179	6		

- Molecule 6 is PALMITIC ACID (three-letter code: PLM) (formula: $C_{16}H_{32}O_2$).

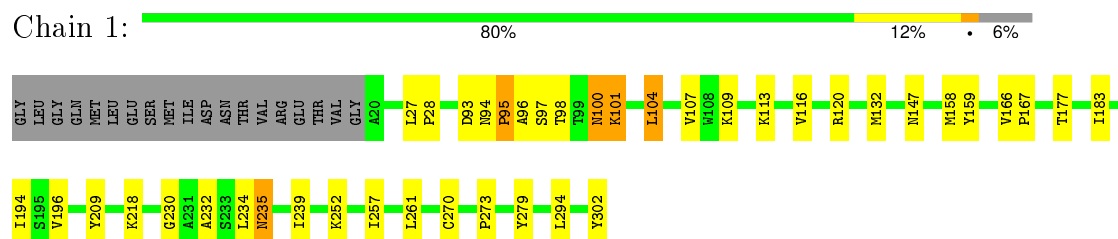


Mol	Chain	Residues	Atoms			AltConf
6	1	1	Total	C	O	0
			14	12	2	

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: Capsid protein VP1



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of images	24717	Depositor
Resolution determination method	FSC 0.143	Depositor
CTF correction method	per particle	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	25	Depositor
Minimum defocus (nm)	-1400	Depositor
Maximum defocus (nm)	-4000	Depositor
Magnification	23000	Depositor
Image detector	GATAN K2 (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: PLM, MYR

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	1	0.57	0/2284	0.95	4/3124 (0.1%)
2	2	0.55	0/2132	0.93	0/2916
3	3	0.53	0/1881	0.97	1/2562 (0.0%)
4	4	0.59	0/528	0.98	1/714 (0.1%)
5	7	0.66	0/943	0.92	1/1278 (0.1%)
All	All	0.57	0/7768	0.95	7/10594 (0.1%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	7	51	LEU	CA-CB-CG	6.95	131.29	115.30
3	3	85	LEU	CA-CB-CG	6.41	130.05	115.30
4	4	21	GLY	N-CA-C	5.45	126.72	113.10
1	1	261	LEU	CA-CB-CG	5.36	127.62	115.30
1	1	234	LEU	CA-CB-CG	5.27	127.42	115.30
1	1	97	SER	N-CA-C	-5.16	97.07	111.00
1	1	104	LEU	CA-CB-CG	5.07	126.95	115.30

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	1	2221	0	2173	40	0
2	2	2075	0	1994	13	0
3	3	1834	0	1816	28	0
4	4	534	0	524	9	0
5	7	921	0	870	20	0
6	1	14	0	20	9	0
All	All	7599	0	7397	101	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 (101) 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)
4:4:20:TYR:CD2	4:4:21:GLY:N	2.35	0.93
4:4:20:TYR:HD2	4:4:21:GLY:H	1.17	0.88
5:7:31:ALA:HB1	5:7:96:TYR:HB2	1.63	0.81
1:1:235:ASN:HD22	1:1:235:ASN:H	1.28	0.79
5:7:50:VAL:HG21	5:7:68:ILE:HB	1.67	0.76
1:1:194:ILE:CD1	6:1:901:PLM:HB1	2.17	0.74
1:1:196:VAL:HG21	6:1:901:PLM:H71	1.69	0.74
5:7:13:GLN:HA	5:7:119:SER:HB3	1.69	0.74
5:7:32:ASN:HD22	5:7:32:ASN:H	1.33	0.73
1:1:183:ILE:HD11	1:1:194:ILE:HD13	1.71	0.71
1:1:101:LYS:NZ	1:1:101:LYS:HA	2.05	0.71
3:3:198:ILE:HG21	3:3:208:MET:CE	2.21	0.70
1:1:232:ALA:O	1:1:235:ASN:ND2	2.24	0.70
5:7:66:PHE:HD2	5:7:79:LEU:HD11	1.57	0.68
5:7:32:ASN:HD22	5:7:32:ASN:N	1.90	0.68
1:1:109:LYS:HA	1:1:239:ILE:HG22	1.75	0.68
2:2:148:ALA:HA	2:2:174:PHE:CE2	2.30	0.66
2:2:148:ALA:HA	2:2:174:PHE:HE2	1.62	0.64
1:1:194:ILE:HD12	6:1:901:PLM:HB1	1.79	0.64
2:2:118:HIS:CD2	2:2:239:PHE:HB2	2.33	0.63
5:7:68:ILE:CD1	5:7:79:LEU:HD13	2.28	0.63
4:4:57:ILE:HD11	4:4:61:LEU:HB2	1.81	0.62
3:3:198:ILE:HG21	3:3:208:MET:HE1	1.82	0.62
3:3:6:ASN:HD22	3:3:6:ASN:H	1.48	0.61
5:7:66:PHE:CD2	5:7:79:LEU:HD11	2.36	0.61
1:1:94:ASN:O	1:1:252:LYS:HD2	2.01	0.60
5:7:68:ILE:HD11	5:7:79:LEU:HD13	1.84	0.60
3:3:87:LEU:HD11	3:3:114:LEU:HD12	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:302:TYR:CE1	3:3:189:TYR:HB3	2.37	0.59
1:1:159:TYR:CD2	6:1:901:PLM:HA2	2.37	0.59
3:3:64:THR:O	3:3:67:MET:HG2	2.02	0.59
1:1:218:LYS:HG3	2:2:269:PRO:O	2.02	0.59
2:2:192:VAL:HG11	3:3:99:MET:HE2	1.87	0.57
3:3:208:MET:N	3:3:208:MET:SD	2.78	0.57
3:3:6:ASN:N	3:3:6:ASN:HD22	2.02	0.57
1:1:94:ASN:H	1:1:252:LYS:HE3	1.70	0.57
1:1:235:ASN:N	1:1:235:ASN:HD22	1.98	0.55
1:1:196:VAL:HG21	6:1:901:PLM:C7	2.36	0.55
1:1:101:LYS:HZ3	1:1:101:LYS:HA	1.69	0.55
1:1:159:TYR:CD2	6:1:901:PLM:H81	2.42	0.55
4:4:22:GLY:O	4:4:24:THR:N	2.40	0.54
3:3:72:LEU:HB2	3:3:208:MET:HE2	1.90	0.53
5:7:107:PHE:CD2	5:7:109:SER:O	2.61	0.53
1:1:100:ASN:HD22	1:1:100:ASN:N	2.07	0.53
5:7:50:VAL:CG2	5:7:68:ILE:HB	2.38	0.52
1:1:116:VAL:CG2	3:3:233:GLN:HB2	2.39	0.52
4:4:20:TYR:CG	4:4:21:GLY:N	2.65	0.52
1:1:120:ARG:HA	1:1:279:TYR:OH	2.09	0.52
1:1:94:ASN:HB2	1:1:252:LYS:HG3	1.92	0.52
3:3:198:ILE:HG21	3:3:208:MET:HE3	1.89	0.52
1:1:116:VAL:HG22	3:3:233:GLN:HB2	1.92	0.51
5:7:39:GLN:HB3	5:7:44:ARG:HA	1.92	0.51
3:3:156:TRP:CD1	3:3:164:CYS:HB2	2.46	0.50
1:1:98:THR:O	1:1:100:ASN:N	2.38	0.50
3:3:85:LEU:HD21	3:3:95:LEU:HD11	1.93	0.50
3:3:55:PHE:HE2	3:3:212:GLY:HA3	1.77	0.49
5:7:86:PRO:HA	5:7:118:VAL:HB	1.94	0.49
3:3:9:GLY:O	3:3:12:GLN:HG2	2.12	0.49
5:7:53:GLY:HA2	5:7:54:GLY:HA2	1.58	0.48
4:4:16:SER:HB3	4:4:20:TYR:HB3	1.94	0.48
3:3:109:HIS:HB3	3:3:176:TYR:HB3	1.95	0.48
1:1:294:LEU:HD11	2:2:186:LEU:HD11	1.95	0.48
1:1:209:TYR:O	1:1:230:GLY:HA2	2.14	0.48
5:7:89:THR:HG23	5:7:117:THR:HA	1.95	0.47
5:7:4:LEU:HD11	5:7:96:TYR:HD1	1.80	0.47
3:3:44:MET:CE	3:3:44:MET:HA	2.44	0.47
3:3:82:ILE:HD12	3:3:192:VAL:HG12	1.97	0.47
1:1:159:TYR:CE2	6:1:901:PLM:H81	2.51	0.46
3:3:90:ALA:HB2	3:3:104:LEU:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:159:TYR:CE2	6:1:901:PLM:H62	2.51	0.45
4:4:20:TYR:HD2	4:4:21:GLY:N	1.96	0.44
4:4:20:TYR:O	4:4:22:GLY:N	2.50	0.44
2:2:74:GLU:N	2:2:74:GLU:CD	2.70	0.44
5:7:20:LEU:HD12	5:7:79:LEU:HD23	2.00	0.44
1:1:239:ILE:C	1:1:239:ILE:HD12	2.38	0.44
5:7:68:ILE:HD13	5:7:79:LEU:HD13	1.99	0.44
2:2:143:THR:HA	2:2:172:ARG:O	2.18	0.43
3:3:6:ASN:N	3:3:6:ASN:ND2	2.66	0.43
5:7:32:ASN:N	5:7:32:ASN:ND2	2.61	0.43
2:2:143:THR:HG23	2:2:173:ARG:HA	2.01	0.43
1:1:132:MET:SD	6:1:901:PLM:H21	2.58	0.43
2:2:201:ARG:NH1	3:3:123:SER:O	2.52	0.43
3:3:234:LYS:HA	3:3:234:LYS:HD3	1.94	0.43
1:1:93:ASP:O	1:1:104:LEU:HG	2.19	0.42
1:1:158:MET:SD	1:1:177:THR:HG22	2.59	0.42
2:2:73:LYS:NZ	2:2:238:ASN:OD1	2.46	0.42
1:1:107:VAL:HG13	1:1:239:ILE:HD13	1.99	0.42
2:2:86:LEU:HD21	2:2:253:ILE:HB	2.01	0.42
3:3:53:ILE:HD11	3:3:214:VAL:HB	2.02	0.41
1:1:101:LYS:HZ2	1:1:101:LYS:HA	1.83	0.41
1:1:257:ILE:HD12	1:1:257:ILE:N	2.36	0.41
1:1:235:ASN:H	1:1:235:ASN:ND2	2.08	0.41
5:7:32:ASN:ND2	5:7:98:ASN:O	2.54	0.41
2:2:64:TYR:CD1	2:2:89:MET:HB3	2.55	0.41
1:1:95:PRO:HB2	1:1:96:ALA:H	1.73	0.41
1:1:27:LEU:HB3	1:1:28:PRO:HD2	2.03	0.41
1:1:166:VAL:HA	1:1:167:PRO:HD2	1.93	0.40
1:1:273:PRO:HA	3:3:99:MET:HE1	2.02	0.40
3:3:45:GLU:OE2	4:4:48:GLN:HG2	2.21	0.40
1:1:100:ASN:N	1:1:100:ASN:ND2	2.69	0.40
3:3:70:VAL:HB	3:3:210:ILE:HG13	2.04	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	1	281/302 (93%)	258 (92%)	20 (7%)	3 (1%)	17	65
2	2	265/272 (97%)	246 (93%)	18 (7%)	1 (0%)	39	80
3	3	233/237 (98%)	225 (97%)	8 (3%)	0	100	100
4	4	66/69 (96%)	52 (79%)	10 (15%)	4 (6%)	2	27
5	7	119/126 (94%)	97 (82%)	17 (14%)	5 (4%)	3	36
All	All	964/1006 (96%)	878 (91%)	73 (8%)	13 (1%)	20	61

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	4	21	GLY
4	4	23	SER
4	4	24	THR
5	7	41	PRO
4	4	19	ALA
5	7	61	SER
5	7	111	GLY
1	1	113	LYS
2	2	48	ASN
1	1	95	PRO
5	7	30	SER
5	7	40	ALA
1	1	270	CYS

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	1	245/261 (94%)	241 (98%)	4 (2%)	70	89
2	2	227/232 (98%)	226 (100%)	1 (0%)	93	97

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	3	210/211 (100%)	207 (99%)	3 (1%)	74	90
4	4	57/57 (100%)	56 (98%)	1 (2%)	66	88
5	7	95/100 (95%)	94 (99%)	1 (1%)	80	92
All	All	834/861 (97%)	824 (99%)	10 (1%)	79	91

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	100	ASN
1	1	101	LYS
1	1	147	ASN
1	1	235	ASN
2	2	74	GLU
3	3	6	ASN
3	3	208	MET
3	3	218	ASN
4	4	18	ARG
5	7	32	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	62	GLN
1	1	100	ASN
1	1	117	GLN
1	1	146	ASN
1	1	235	ASN
2	2	48	ASN
2	2	111	GLN
2	2	165	ASN
2	2	272	GLN
3	3	6	ASN
3	3	97	HIS
3	3	105	ASN
3	3	218	ASN
4	4	31	ASN
5	7	3	GLN
5	7	32	ASN
5	7	39	GLN

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 ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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	$\# Z > 2$
6	PLM	1	901	-	10,13,17	0.35	0	10,13,17	0.46	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
6	PLM	1	901	-	-	0/9/11/15	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	1	901	PLM	9	0

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.