wwPDB EM Validation Summary Report (i)

Feb 22, 2024 – 03:18 AM JST

PDB ID	:	8JXQ
EMDB ID	:	EMD-36709
Title	:	Cryo-EM structure of bilirubin ditaurate (BDT) bound human ABC transporter ABCC2
Authors	:	Mao, Y.X.; Chen, Z.P.; Wang, L.; Hou, W.T.; Chen, Y.X.; Zhou, C.Z.
Deposited on	:	2023-07-01
Resolution	:	3.32 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 (i) symbol.

The types of validation reports are described at
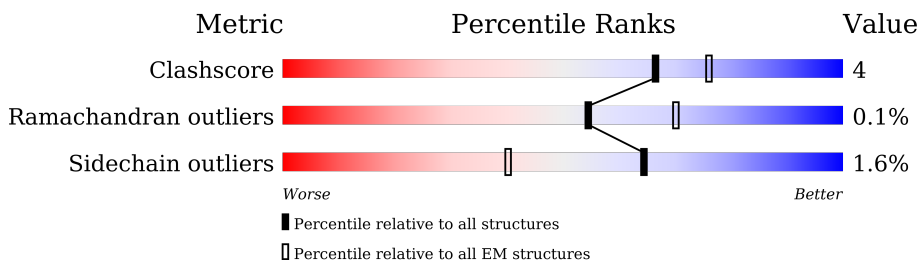http://www.wwpdb.org/validation/2017/FAQs#types.

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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 3.32 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	Percentile Ranks	Value
Clashscore		4
Ramachandran outliers		0.1%
Sidechain outliers		1.6%

Worse ... *Better*

▌ Percentile relative to all structures
▯ Percentile relative to all EM structures

Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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 <=5%

Mol	Chain	Length	Quality of chain
1	A	1565	79% 10% 11%

2   Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 22443 atoms, of which 11333 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 ATP-binding cassette sub-family C member 2.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
1	A	1388	22314	7164	11287	1823	1983	57	0	0

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1546	LEU	-	expression tag	UNP Q92887
A	1547	GLU	-	expression tag	UNP Q92887
A	1548	ASP	-	expression tag	UNP Q92887
A	1549	TYR	-	expression tag	UNP Q92887
A	1550	LYS	-	expression tag	UNP Q92887
A	1551	ASP	-	expression tag	UNP Q92887
A	1552	ASP	-	expression tag	UNP Q92887
A	1553	ASP	-	expression tag	UNP Q92887
A	1554	ASP	-	expression tag	UNP Q92887
A	1555	LYS	-	expression tag	UNP Q92887
A	1556	VAL	-	expression tag	UNP Q92887
A	1557	GLU	-	expression tag	UNP Q92887
A	1558	HIS	-	expression tag	UNP Q92887
A	1559	HIS	-	expression tag	UNP Q92887
A	1560	HIS	-	expression tag	UNP Q92887
A	1561	HIS	-	expression tag	UNP Q92887
A	1562	HIS	-	expression tag	UNP Q92887
A	1563	HIS	-	expression tag	UNP Q92887
A	1564	HIS	-	expression tag	UNP Q92887
A	1565	HIS	-	expression tag	UNP Q92887

- Molecule 2 is CHOLESTEROL (three-letter code: CLR) (formula: $C_{27}H_{46}O$) (labeled as "Ligand of Interest" by depositor).
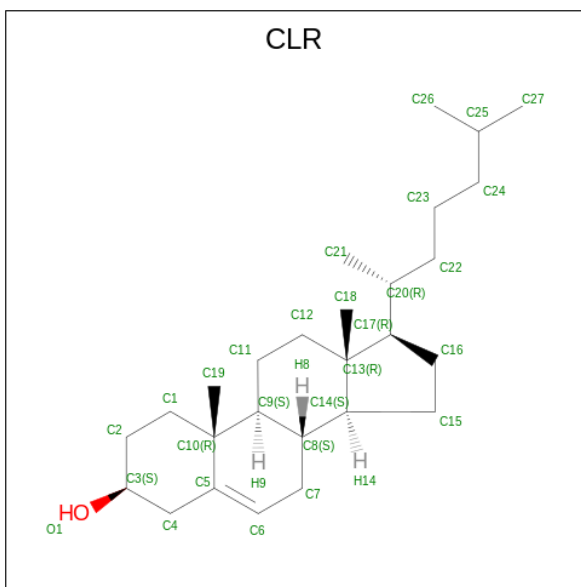
Mol	Chain	Residues	Atoms				AltConf
			Total	C	H	O	
2	A	1	74	27	46	1	0

- Molecule 3 is 2-[3-[5-[(E)-(4-ethenyl-3-methyl-5-oxidanylidene-pyrrol-2-ylidene)methyl]-2-[[5-[(3-ethenyl-4-methyl-5-oxidanylidene-pyrrol-2-ylidene)methyl]-4-methyl-3-[3-oxidanylid ene-3-(2-sulfoethylamino)propyl]-1H-pyrrol-2-yl]methyl]-4-methyl-1H-pyrrol-3-yl]propano ylamino]ethanesulfonic acid (three-letter code: FEI) (formula: $C_{37}H_{46}N_6O_{10}S_2$) (labeled as "Ligand of Interest" by depositor).
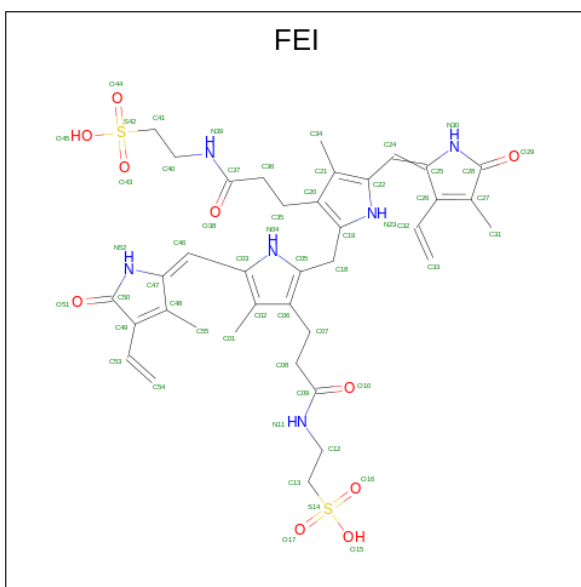
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	S	
3	A	1	55	37	6	10	2	0

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: ATP-binding cassette sub-family C member 2

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	368404	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 $(e^-/\text{Å}^2)$	55	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2000	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: CLR, FEI

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	0.25	0/11262	0.45	0/15272

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 ⓘ

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	11027	11287	11287	89	0
2	A	28	46	46	0	0
3	A	55	0	0	2	0
All	All	11110	11333	11333	89	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 4.

The worst 5 of 89 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:810:LEU:O	1:A:815:ARG:NH1	2.09	0.86

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W O R L D W I D E
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PROTEIN DATA BANK

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1308:ARG:NH1	1:A:1313:LEU:O	2.09	0.85
1:A:1097:GLN:O	1:A:1097:GLN:NE2	2.16	0.79
1:A:661:ILE:CD1	1:A:667:VAL:HG21	2.15	0.77
1:A:800:PHE:O	1:A:805:GLY:N	2.21	0.74

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	A	1380/1565 (88%)	1359 (98%)	20 (1%)	1 (0%)	51	81

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	191	SER

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	1230/1392 (88%)	1210 (98%)	20 (2%)	62	80

5 of 20 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1083	ARG
1	A	1308	ARG
1	A	1403	ASP
1	A	1372	ASP
1	A	462	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	#$|Z| > 2$
3	FEI	A	1602	-	52,58,58	3.54	23 (44%)	60,85,85	2.35	18 (30%)
2	CLR	A	1601	-	31,31,31	0.37	0	48,48,48	0.79	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
3	FEI	A	1602	-	-	16/38/72/72	0/4/4/4
2	CLR	A	1601	-	-	4/10/68/68	0/4/4/4

The worst 5 of 23 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1602	FEI	C24-C25	9.01	1.53	1.34
3	A	1602	FEI	C46-C47	9.01	1.53	1.34
3	A	1602	FEI	O29-C28	8.85	1.40	1.23
3	A	1602	FEI	O51-C50	8.64	1.40	1.23
3	A	1602	FEI	C37-N39	5.46	1.45	1.33

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1602	FEI	O16-S14-C13	7.17	115.55	106.92
3	A	1602	FEI	O43-S42-C41	6.12	114.28	106.92
3	A	1602	FEI	O17-S14-C13	6.01	114.15	106.92
3	A	1602	FEI	O44-S42-C41	5.54	113.59	106.92
3	A	1602	FEI	O45-S42-C41	5.43	114.54	105.77

There are no chirality outliers.

5 of 20 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1602	FEI	C22-C24-C25-C26
3	A	1602	FEI	C22-C24-C25-N30
3	A	1602	FEI	C06-C07-C08-C09
3	A	1602	FEI	C40-C41-S42-O43
3	A	1602	FEI	C40-C41-S42-O44

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1602	FEI	2	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 then 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.

Ligand FEI A 1602

Bond lengths

Bond angles

Torsions

Rings

Ligand CLR A 1601	

Bond lengths |

Bond angles |
|

Torsions |

Rings |
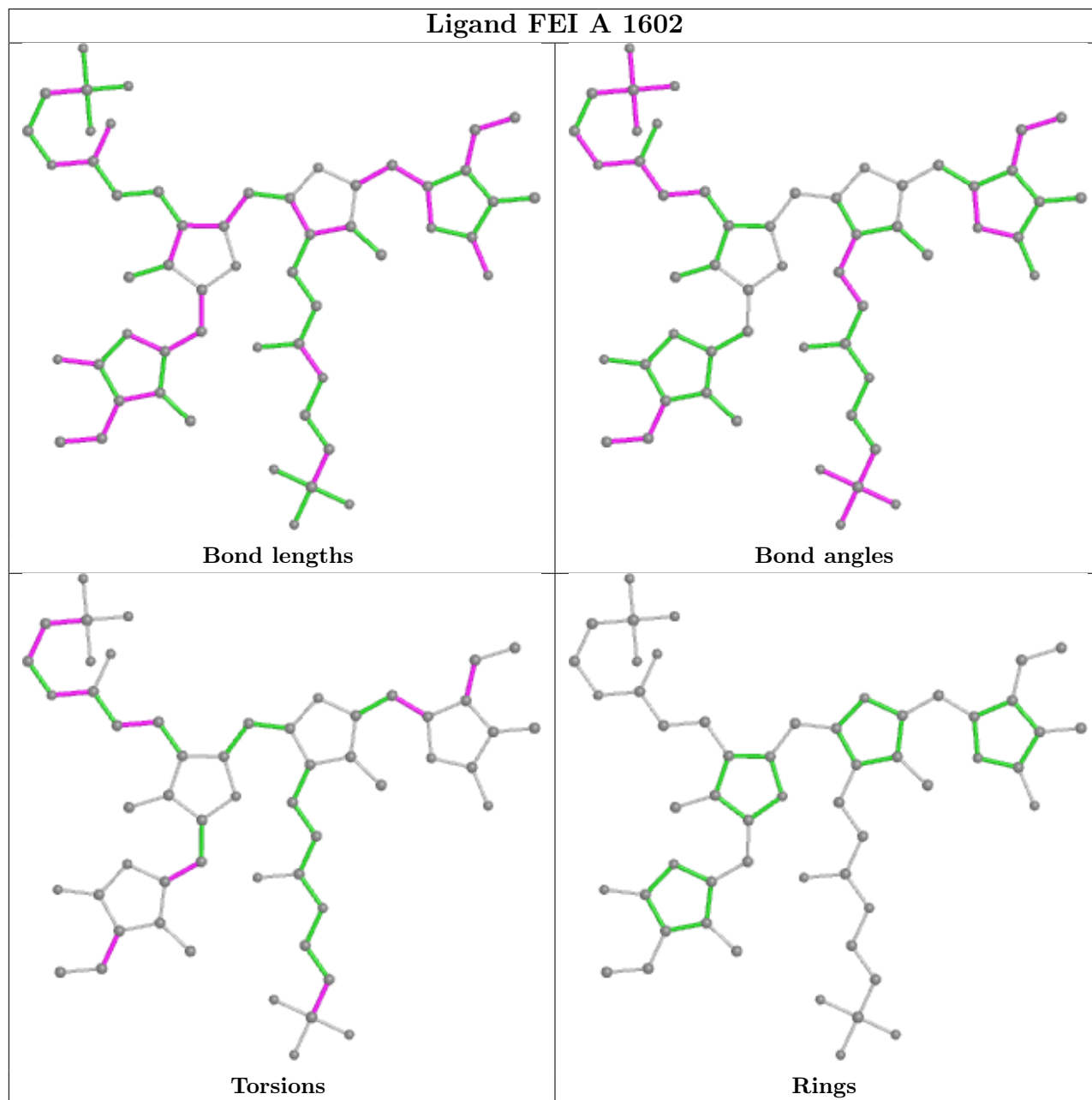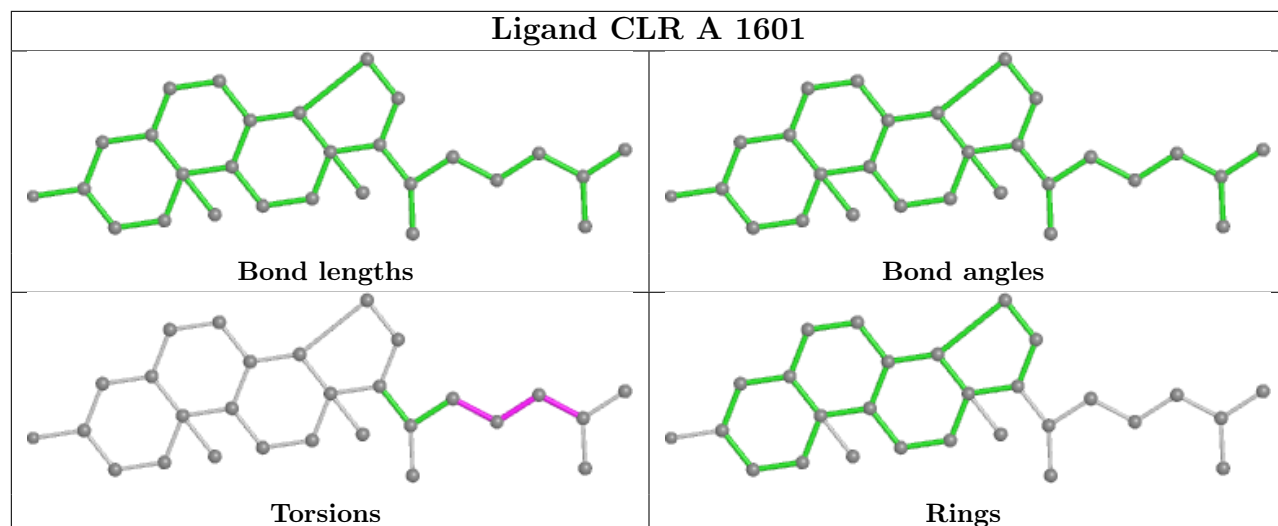
5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.