



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

Feb 3, 2018 – 11:28 PM EST

PDB ID : 6EQC  
EMDB ID: : EMD-3821  
Title : Cryo-EM reconstruction of a complex of a binding protein and human adenovirus C5 hexon  
Authors : Schmid, M.; Ernst, P.; Honegger, A.; Suomalainen, M.; Zimmermann, M.; Braun, L.; Stauffer, S.; Thom, C.; Dreier, B.; Eibauer, M.; Kipar, A.; Vogel, V.; Greber, U.F.; Medalia, O.; Plueckthun, A.  
Deposited on : 2017-10-12  
Resolution : 7.40 Å(reported)

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  
<http://wwpdb.org/validation/2016/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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MolProbity : 4.02b-467  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20030736

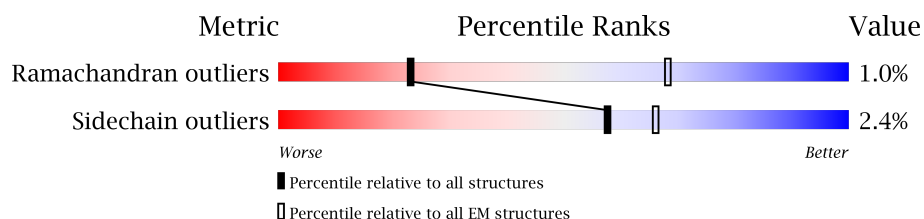
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 7.40 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)
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026

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	952	
1	B	952	
1	C	952	
2	D	254	
2	E	254	
2	F	254	

## 2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 53964 atoms, of which 26442 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 Hexon protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	921	Total	C	H	N	O	S	0	0
			14445	4686	7070	1250	1404	35		
1	B	921	Total	C	H	N	O	S	0	0
			14445	4686	7070	1250	1404	35		
1	C	921	Total	C	H	N	O	S	0	0
			14445	4686	7070	1250	1404	35		

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	272	ALA	THR	conflict	UNP P04133
A	420	GLY	ILE	conflict	UNP P04133
A	422	ASN	THR	conflict	UNP P04133
A	423	SER	GLU	conflict	UNP P04133
A	425	TYR	LEU	conflict	UNP P04133
B	272	ALA	THR	conflict	UNP P04133
B	420	GLY	ILE	conflict	UNP P04133
B	422	ASN	THR	conflict	UNP P04133
B	423	SER	GLU	conflict	UNP P04133
B	425	TYR	LEU	conflict	UNP P04133
C	272	ALA	THR	conflict	UNP P04133
C	420	GLY	ILE	conflict	UNP P04133
C	422	ASN	THR	conflict	UNP P04133
C	423	SER	GLU	conflict	UNP P04133
C	425	TYR	LEU	conflict	UNP P04133

- Molecule 2 is a protein called scFv of 9C12 antibody.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	D	233	Total	C	H	N	O	S	0	0
			3543	1130	1744	306	356	7		
2	E	233	Total	C	H	N	O	S	0	0
			3543	1130	1744	306	356	7		

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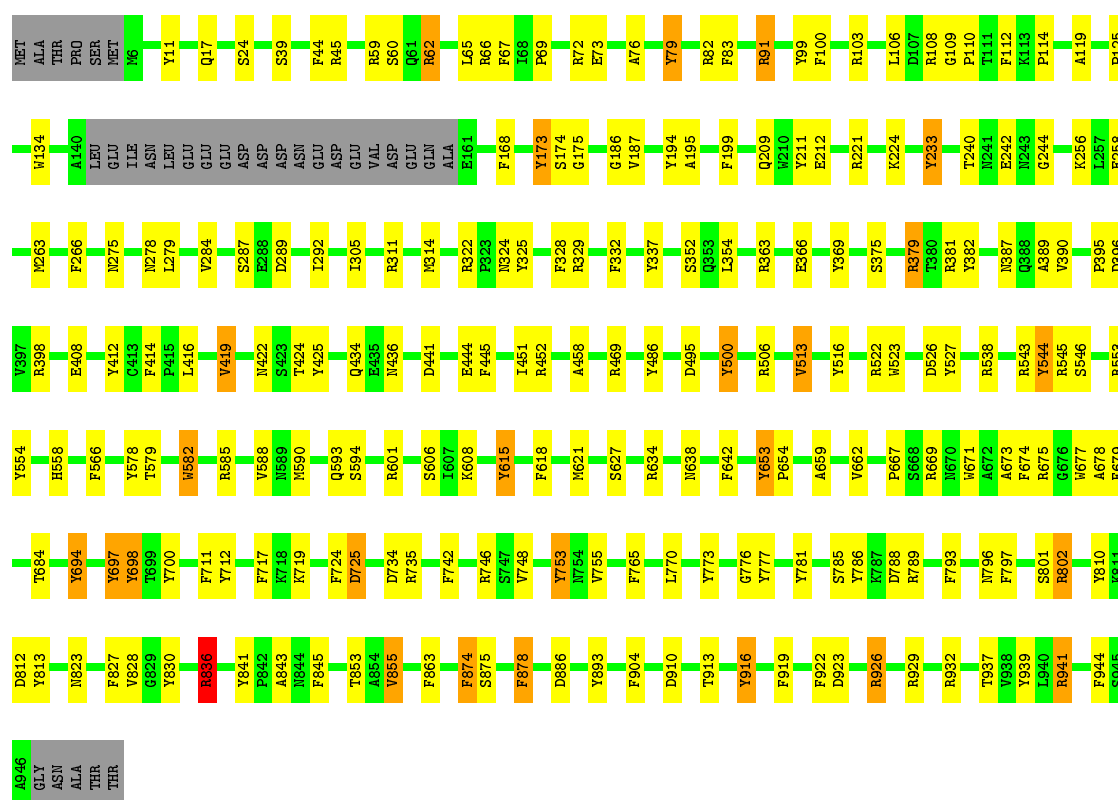
Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
2	F	233	3543	1130	1744	306	356	7	0	0

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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.

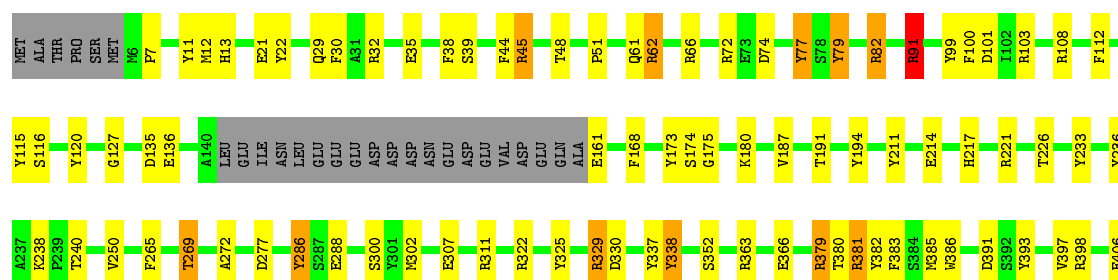
- Molecule 1: Hexon protein

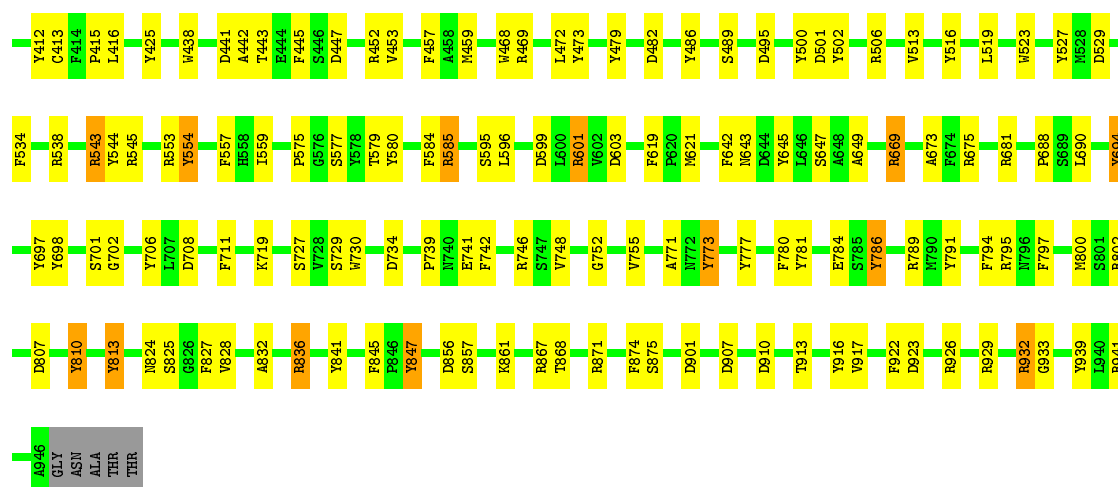
Chain A: 



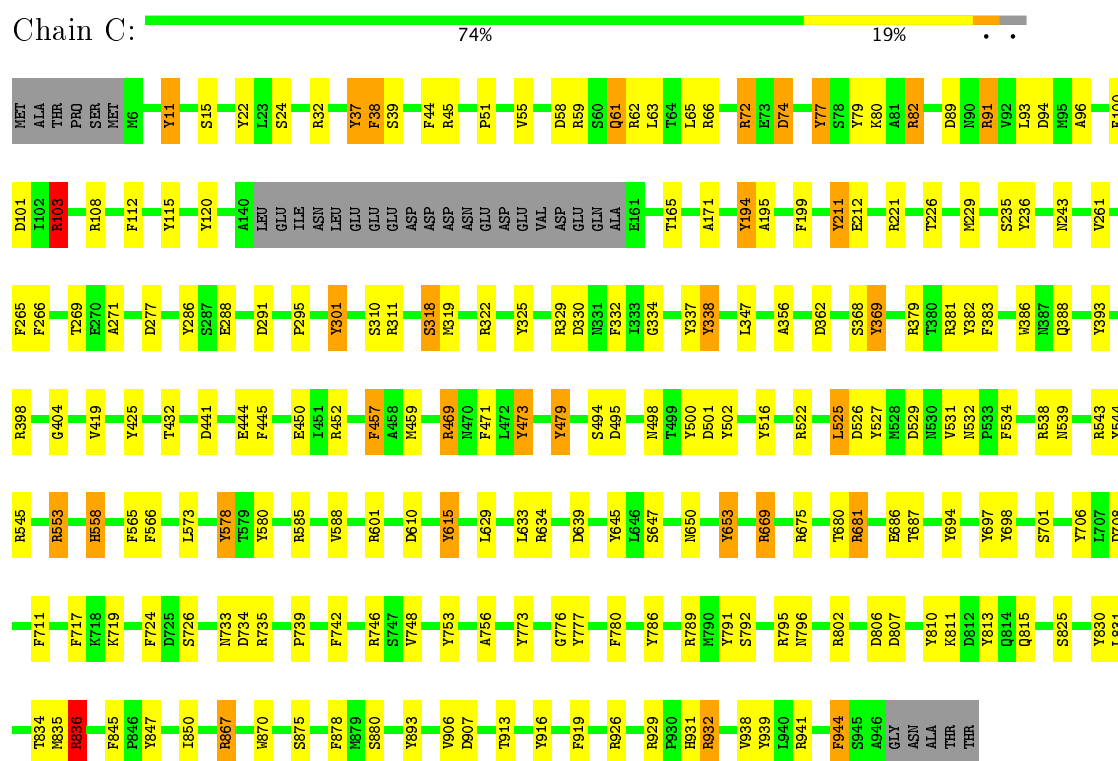
- Molecule 1: Hexon protein

Chain B: 

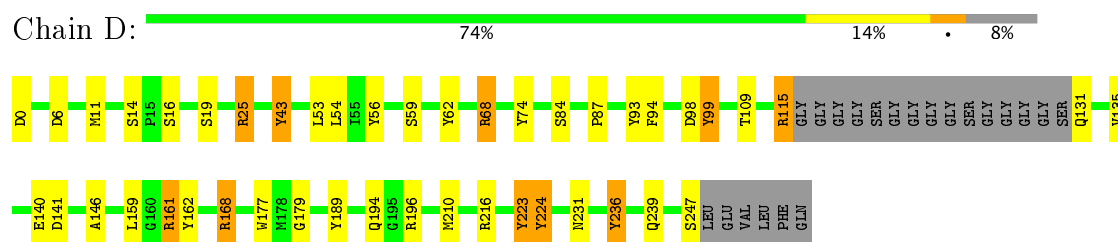




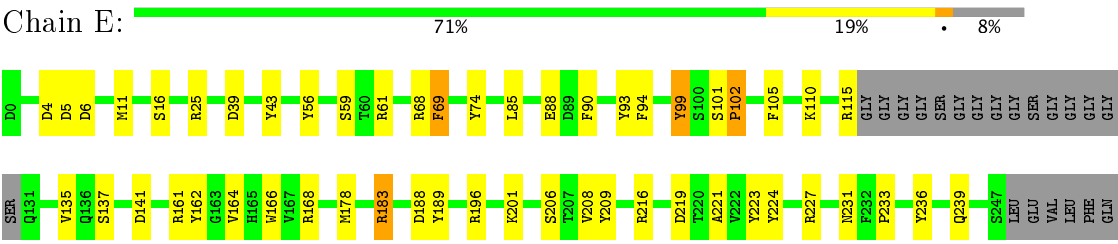
- Molecule 1: Hexon protein



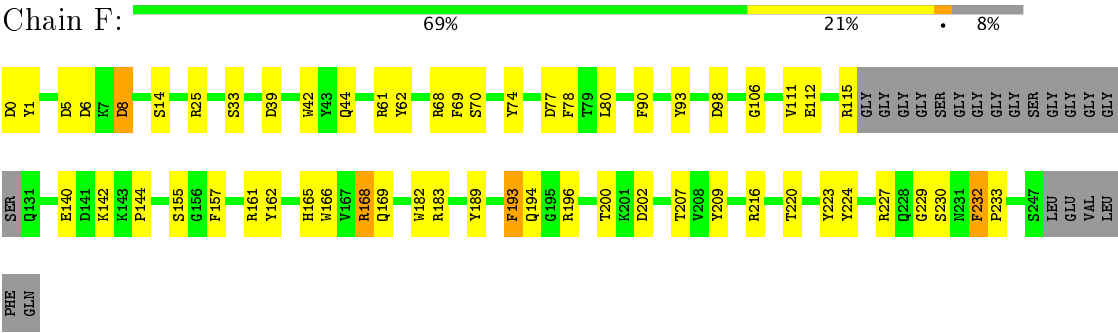
- Molecule 2: scFv of 9C12 antibody



- Molecule 2: scFv of 9C12 antibody



• Molecule 2: scFv of 9C12 antibody



## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	1880	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	1.0	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor



## 5 Model quality

### 5.1 Standard geometry

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	1.66	46/7574 (0.6%)	2.11	221/10299 (2.1%)
1	B	1.65	51/7574 (0.7%)	2.08	228/10299 (2.2%)
1	C	1.66	44/7574 (0.6%)	2.00	218/10299 (2.1%)
2	D	1.73	14/1839 (0.8%)	1.98	50/2490 (2.0%)
2	E	1.71	19/1839 (1.0%)	2.24	53/2490 (2.1%)
2	F	1.75	22/1839 (1.2%)	2.10	55/2490 (2.2%)
All	All	1.67	196/28239 (0.7%)	2.07	825/38367 (2.2%)

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	26
1	B	0	28
1	C	0	33
2	D	0	10
2	E	0	6
2	F	0	4
All	All	0	107

The worst 5 of 196 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	33	SER	CA-CB	8.58	1.65	1.52
1	A	186	GLY	CA-C	8.47	1.65	1.51
2	E	224	TYR	CB-CG	-8.27	1.39	1.51
1	B	21	GLU	CG-CD	7.95	1.63	1.51
1	C	653	TYR	CE2-CZ	7.74	1.48	1.38

The worst 5 of 825 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	363	ARG	NE-CZ-NH2	-27.23	106.68	120.30
2	E	196	ARG	NE-CZ-NH1	26.14	133.37	120.30
2	E	183	ARG	NE-CZ-NH2	-25.28	107.66	120.30
1	B	746	ARG	NE-CZ-NH1	23.92	132.26	120.30
2	F	168	ARG	NE-CZ-NH2	-23.38	108.61	120.30

There are no chirality outliers.

5 of 107 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	173	TYR	Sidechain
1	A	233	TYR	Sidechain
1	A	62	ARG	Sidechain
1	A	79	TYR	Sidechain
1	A	91	ARG	Sidechain

## 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	7375	7070	7068	0	0
1	B	7375	7070	7068	0	0
1	C	7375	7070	7068	0	0
2	D	1799	1744	1743	0	0
2	E	1799	1744	1743	0	0
2	F	1799	1744	1743	0	0
All	All	27522	26442	26433	0	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). Clashscore could not be calculated for this entry.

There are no clashes within the asymmetric unit.

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	917/952 (96%)	866 (94%)	43 (5%)	8 (1%)	20	63
1	B	917/952 (96%)	863 (94%)	47 (5%)	7 (1%)	22	67
1	C	917/952 (96%)	853 (93%)	51 (6%)	13 (1%)	13	54
2	D	229/254 (90%)	213 (93%)	15 (7%)	1 (0%)	38	77
2	E	229/254 (90%)	207 (90%)	18 (8%)	4 (2%)	11	50
2	F	229/254 (90%)	211 (92%)	16 (7%)	2 (1%)	20	63
All	All	3438/3618 (95%)	3213 (94%)	190 (6%)	35 (1%)	23	61

5 of 35 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	295	PRO
1	C	539	ASN
2	E	231	ASN
1	C	61	GLN
1	C	734	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	800/827 (97%)	780 (98%)	20 (2%)	53	77
1	B	800/827 (97%)	775 (97%)	25 (3%)	45	71
1	C	800/827 (97%)	778 (97%)	22 (3%)	49	74

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	D	197/206 (96%)	196 (100%)	1 (0%)	91	95
2	E	197/206 (96%)	195 (99%)	2 (1%)	80	90
2	F	197/206 (96%)	194 (98%)	3 (2%)	70	85
All	All	2991/3099 (96%)	2918 (98%)	73 (2%)	58	78

5 of 73 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	643	ASN
1	B	836	ARG
2	D	239	GLN
1	B	741	GLU
1	B	861	LYS

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

### 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](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.