



# Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Dec 8, 2019 – 10:49 PM EST

PDB ID : 6RVX  
EMDB ID: : EMD-10016  
Title : Inward-open structure of the ASCT2 (SLC1A5) mutant C467R in presence of TBOA  
Authors : Garaeva, A.A.; Guskov, A.; Slotboom, D.J.; Paulino, C.  
Deposited on : 2019-06-03  
Resolution : 3.61 Å(reported)  
Based on PDB ID : 6GCT

This is a Full wwPDB/EMDatabank EM Map/Model Validation 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  
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

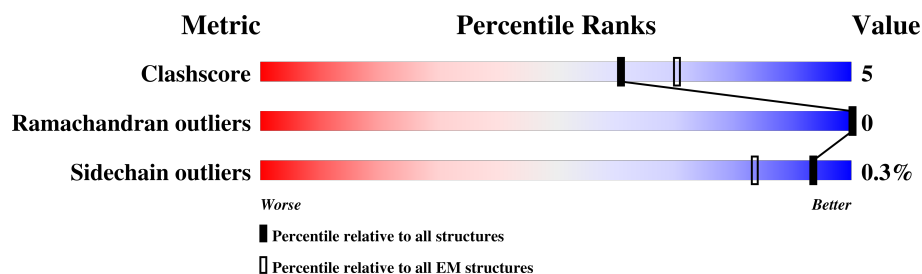
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.61 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	547	69% 10% 21%
1	B	547	68% 11% 21%
1	C	547	69% 10% 21%

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 9627 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 Neutral amino acid transporter B(0).

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	430	Total	C	N	O	S	0	0
			3209	2100	534	560	15		
1	B	430	Total	C	N	O	S	0	0
			3209	2100	534	560	15		
1	C	430	Total	C	N	O	S	0	0
			3209	2100	534	560	15		

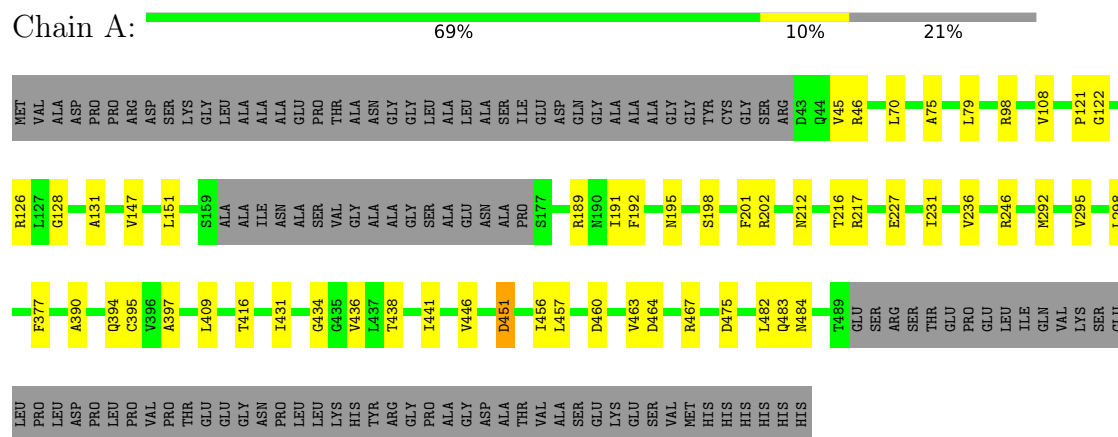
There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	467	ARG	CYS	engineered mutation	UNP Q15758
A	542	HIS	-	expression tag	UNP Q15758
A	543	HIS	-	expression tag	UNP Q15758
A	544	HIS	-	expression tag	UNP Q15758
A	545	HIS	-	expression tag	UNP Q15758
A	546	HIS	-	expression tag	UNP Q15758
A	547	HIS	-	expression tag	UNP Q15758
B	467	ARG	CYS	engineered mutation	UNP Q15758
B	542	HIS	-	expression tag	UNP Q15758
B	543	HIS	-	expression tag	UNP Q15758
B	544	HIS	-	expression tag	UNP Q15758
B	545	HIS	-	expression tag	UNP Q15758
B	546	HIS	-	expression tag	UNP Q15758
B	547	HIS	-	expression tag	UNP Q15758
C	467	ARG	CYS	engineered mutation	UNP Q15758
C	542	HIS	-	expression tag	UNP Q15758
C	543	HIS	-	expression tag	UNP Q15758
C	544	HIS	-	expression tag	UNP Q15758
C	545	HIS	-	expression tag	UNP Q15758
C	546	HIS	-	expression tag	UNP Q15758
C	547	HIS	-	expression tag	UNP Q15758

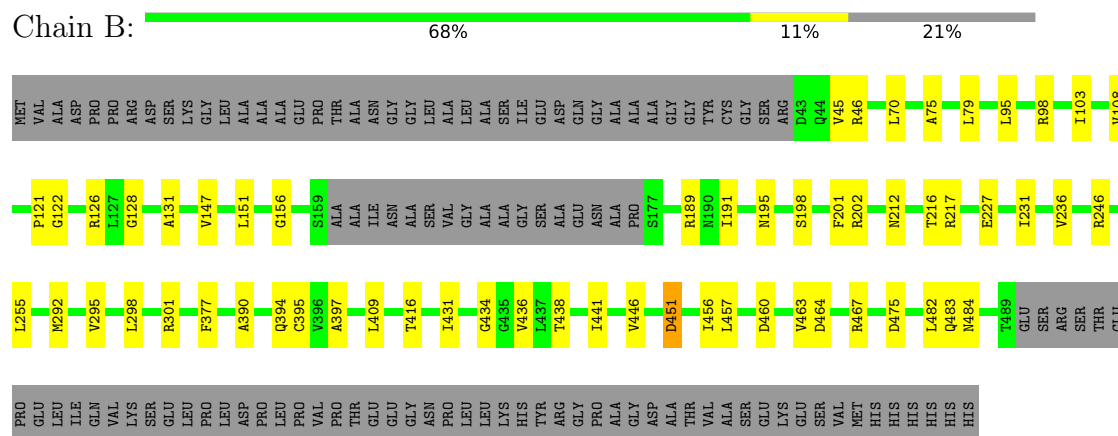
### 3 Residue-property plots

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.

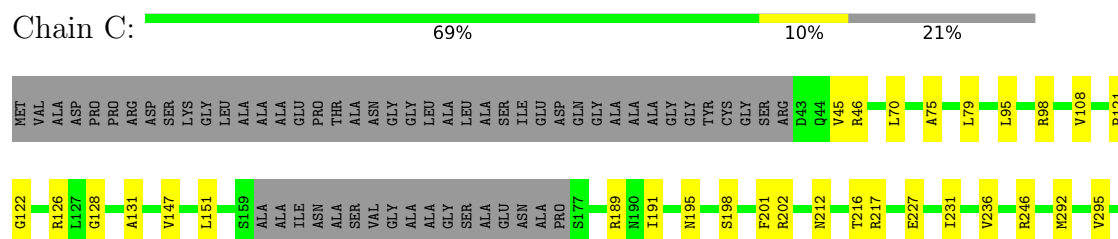
#### • Molecule 1: Neutral amino acid transporter B(0)



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L298	GLU
F377	LEU
A390	PRO
Q394	LEU
C395	PRO
V396	VAL
A397	PRO
	THR
L409	GLU
T416	GLY
	ASN
I431	PRO
	LEU
G434	LEU
G435	LYS
V436	HIS
L437	TYR
T438	ARG
	GLY
I441	PRO
V446	GLY
D451	ASP
	ALA
T456	THR
L457	VAL
	ALA
D460	SER
V463	GLU
D464	LYS
	GLU
R467	SER
	VAL
D475	MET
	HIS
L482	HIS
Q483	HIS
I484	HIS
T489	HIS
GLU	GLU
SER	SER
ARG	ARG
SER	SER
THR	THR
GLU	GLU
PRO	PRO
GLU	GLU
LEU	LEU
ILE	ILE
GLN	GLN
VAL	VAL
LYS	LYS
SER	SER

GLU
LEU
PRO
LEU
ASP
PRO
LEU
PRO
VAL
PRO
THR
GLU
GLY
ASN
PRO
LEU
LYS
HIS
TYR
ARG
GLY
PRO
ALA
GLY
ASP
ALA
THR
VAL
ALA
SER
GLU
LYS
GLU
SER
VAL
MET
HIS
HIS
HIS
HIS
HIS

## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	223354	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	52	Depositor
Minimum defocus (nm)	300	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	49407	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	0.32	0/3266	0.55	0/4448
1	B	0.32	0/3266	0.55	0/4448
1	C	0.32	0/3266	0.55	0/4448
All	All	0.32	0/9798	0.55	0/13344

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	3209	0	3385	35	0
1	B	3209	0	3385	39	0
1	C	3209	0	3385	35	0
All	All	9627	0	10155	99	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 5.

All (99) 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:B:122:GLY:HA3	1:B:126:ARG:HE	1.61	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:122:GLY:HA3	1:C:126:ARG:HE	1.61	0.66
1:A:122:GLY:HA3	1:A:126:ARG:HE	1.61	0.64
1:A:436:VAL:HG21	1:A:457:LEU:HD13	1.85	0.59
1:B:436:VAL:HG21	1:B:457:LEU:HD13	1.85	0.59
1:C:436:VAL:HG21	1:C:457:LEU:HD13	1.85	0.59
1:A:397:ALA:HB1	1:A:456:ILE:HD13	1.86	0.58
1:C:397:ALA:HB1	1:C:456:ILE:HD13	1.86	0.57
1:B:397:ALA:HB1	1:B:456:ILE:HD13	1.86	0.57
1:A:202:ARG:NH1	1:B:227:GLU:OE1	2.37	0.56
1:B:195:ASN:HD21	1:C:201:PHE:HB3	1.69	0.56
1:C:436:VAL:HG11	1:C:457:LEU:HD22	1.88	0.55
1:A:195:ASN:HD21	1:B:201:PHE:HB3	1.70	0.55
1:A:436:VAL:HG11	1:A:457:LEU:HD22	1.88	0.55
1:C:475:ASP:OD1	1:C:475:ASP:N	2.40	0.55
1:B:436:VAL:HG11	1:B:457:LEU:HD22	1.88	0.54
1:B:216:THR:HG23	1:B:217:ARG:HG2	1.90	0.54
1:C:390:ALA:O	1:C:394:GLN:NE2	2.41	0.54
1:A:216:THR:HG23	1:A:217:ARG:HG2	1.90	0.53
1:A:390:ALA:O	1:A:394:GLN:NE2	2.41	0.53
1:A:475:ASP:N	1:A:475:ASP:OD1	2.40	0.53
1:B:390:ALA:O	1:B:394:GLN:NE2	2.41	0.53
1:A:483:GLN:NE2	1:A:484:ASN:OD1	2.42	0.52
1:C:212:ASN:ND2	1:C:216:THR:O	2.42	0.52
1:C:216:THR:HG23	1:C:217:ARG:HG2	1.90	0.52
1:B:189:ARG:O	1:C:98:ARG:NH2	2.38	0.52
1:B:463:VAL:O	1:B:467:ARG:HB2	2.10	0.52
1:C:438:THR:HA	1:C:441:ILE:HD12	1.92	0.52
1:A:189:ARG:O	1:B:98:ARG:NH2	2.36	0.52
1:B:483:GLN:NE2	1:B:484:ASN:OD1	2.43	0.52
1:C:463:VAL:O	1:C:467:ARG:HB2	2.10	0.51
1:C:483:GLN:NE2	1:C:484:ASN:OD1	2.43	0.51
1:A:463:VAL:O	1:A:467:ARG:HB2	2.10	0.51
1:A:438:THR:HA	1:A:441:ILE:HD12	1.92	0.51
1:B:212:ASN:ND2	1:B:216:THR:O	2.42	0.50
1:B:438:THR:HA	1:B:441:ILE:HD12	1.92	0.50
1:A:212:ASN:ND2	1:A:216:THR:O	2.42	0.49
1:B:475:ASP:N	1:B:475:ASP:OD1	2.40	0.49
1:A:201:PHE:HB3	1:C:195:ASN:HD21	1.77	0.49
1:C:75:ALA:HB1	1:C:79:LEU:HB2	1.94	0.49
1:A:416:THR:HG23	1:A:446:VAL:HG12	1.94	0.49
1:A:75:ALA:HB1	1:A:79:LEU:HB2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:202:ARG:NH1	1:C:227:GLU:OE1	2.44	0.49
1:A:460:ASP:O	1:A:464:ASP:HB2	2.13	0.49
1:A:121:PRO:HD3	1:A:246:ARG:HD2	1.95	0.48
1:B:416:THR:HG23	1:B:446:VAL:HG12	1.94	0.48
1:C:460:ASP:O	1:C:464:ASP:HB2	2.13	0.48
1:B:75:ALA:HB1	1:B:79:LEU:HB2	1.94	0.48
1:B:121:PRO:HD3	1:B:246:ARG:HD2	1.95	0.48
1:C:121:PRO:HD3	1:C:246:ARG:HD2	1.95	0.48
1:C:416:THR:HG23	1:C:446:VAL:HG12	1.94	0.47
1:A:147:VAL:HG23	1:A:395:CYS:HB3	1.97	0.47
1:B:460:ASP:O	1:B:464:ASP:HB2	2.13	0.47
1:C:198:SER:OG	1:C:198:SER:O	2.32	0.47
1:B:147:VAL:HG23	1:B:395:CYS:HB3	1.97	0.45
1:A:198:SER:OG	1:A:202:ARG:NE	2.47	0.45
1:C:431:ILE:HB	1:C:434:GLY:HA2	1.99	0.45
1:A:451:ASP:OD1	1:A:451:ASP:N	2.50	0.45
1:C:147:VAL:HG23	1:C:395:CYS:HB3	1.97	0.45
1:B:292:MET:HG3	1:B:298:LEU:HD13	1.99	0.45
1:C:292:MET:HG3	1:C:298:LEU:HD13	1.99	0.45
1:A:292:MET:HG3	1:A:298:LEU:HD13	1.99	0.45
1:B:128:GLY:HA3	1:B:377:PHE:HE2	1.82	0.45
1:C:451:ASP:OD1	1:C:451:ASP:N	2.50	0.45
1:B:451:ASP:N	1:B:451:ASP:OD1	2.50	0.45
1:A:431:ILE:HB	1:A:434:GLY:HA2	1.98	0.44
1:B:431:ILE:HB	1:B:434:GLY:HA2	1.98	0.44
1:C:128:GLY:HA3	1:C:377:PHE:HE2	1.82	0.44
1:C:70:LEU:HD21	1:C:295:VAL:HG11	2.00	0.44
1:A:128:GLY:HA3	1:A:377:PHE:HE2	1.82	0.44
1:B:70:LEU:HD21	1:B:295:VAL:HG11	2.00	0.44
1:A:70:LEU:HD21	1:A:295:VAL:HG11	2.00	0.43
1:A:45:VAL:HG13	1:A:46:ARG:HG2	2.01	0.43
1:B:45:VAL:HG13	1:B:46:ARG:HG2	2.01	0.43
1:C:45:VAL:HG13	1:C:46:ARG:HG2	2.01	0.43
1:C:108:VAL:HG21	1:C:231:ILE:HG23	2.01	0.42
1:C:95:LEU:HD12	1:C:95:LEU:HA	1.88	0.42
1:A:192:PHE:HD2	1:B:95:LEU:HD11	1.85	0.42
1:A:227:GLU:OE1	1:C:202:ARG:NH1	2.48	0.42
1:B:198:SER:OG	1:B:202:ARG:NE	2.47	0.42
1:A:434:GLY:O	1:A:438:THR:OG1	2.26	0.42
1:B:191:ILE:HG23	1:B:236:VAL:HG21	2.02	0.42
1:C:191:ILE:HG23	1:C:236:VAL:HG21	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:409:LEU:HA	1:B:409:LEU:HD12	1.91	0.42
1:B:108:VAL:HG21	1:B:231:ILE:HG23	2.01	0.42
1:A:108:VAL:HG21	1:A:231:ILE:HG23	2.01	0.41
1:C:198:SER:OG	1:C:202:ARG:NE	2.47	0.41
1:B:103:ILE:HA	1:B:103:ILE:HD13	1.90	0.41
1:A:98:ARG:NH2	1:C:189:ARG:O	2.42	0.41
1:A:191:ILE:HG23	1:A:236:VAL:HG21	2.02	0.41
1:B:95:LEU:HD12	1:B:95:LEU:HA	1.88	0.41
1:C:151:LEU:HD21	1:C:409:LEU:HD23	2.03	0.41
1:B:131:ALA:HB2	1:B:482:LEU:HD22	2.02	0.41
1:B:156:GLY:HA2	1:B:301:ARG:HG2	2.03	0.41
1:A:151:LEU:HD21	1:A:409:LEU:HD23	2.03	0.40
1:B:255:LEU:HD23	1:B:255:LEU:HA	1.90	0.40
1:B:151:LEU:HD21	1:B:409:LEU:HD23	2.03	0.40
1:C:131:ALA:HB2	1:C:482:LEU:HD22	2.02	0.40
1:A:131:ALA:HB2	1:A:482:LEU:HD22	2.02	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	A	426/547 (78%)	392 (92%)	34 (8%)	0	100	100
1	B	426/547 (78%)	392 (92%)	34 (8%)	0	100	100
1	C	426/547 (78%)	392 (92%)	34 (8%)	0	100	100
All	All	1278/1641 (78%)	1176 (92%)	102 (8%)	0	100	100

There are no Ramachandran outliers to report.

### 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	340/425 (80%)	339 (100%)	1 (0%)	93	98
1	B	340/425 (80%)	339 (100%)	1 (0%)	93	98
1	C	340/425 (80%)	339 (100%)	1 (0%)	93	98
All	All	1020/1275 (80%)	1017 (100%)	3 (0%)	93	98

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	451	ASP
1	B	451	ASP
1	C	451	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	313	HIS
1	A	316	HIS
1	A	386	ASN
1	A	394	GLN
1	A	483	GLN
1	B	313	HIS
1	B	316	HIS
1	B	386	ASN
1	B	394	GLN
1	B	483	GLN
1	C	313	HIS
1	C	316	HIS
1	C	386	ASN
1	C	394	GLN
1	C	483	GLN

### 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 [i](#)

There are no chain breaks in this entry.