



# wwPDB X-ray Structure Validation Summary Report

Feb 27, 2014 – 08:32 PM GMT

PDB ID : 2HTK  
Title : Structure of the Escherichia coli ClC chloride channel Y445A mutant and Fab complex  
Authors : Accardi, A.; Lobet, S.; Williams, C.; Miller, C.; Dutzler, R.  
Deposited on : 2006-07-26  
Resolution : 3.41 Å(reported)

This is a wwPDB validation summary report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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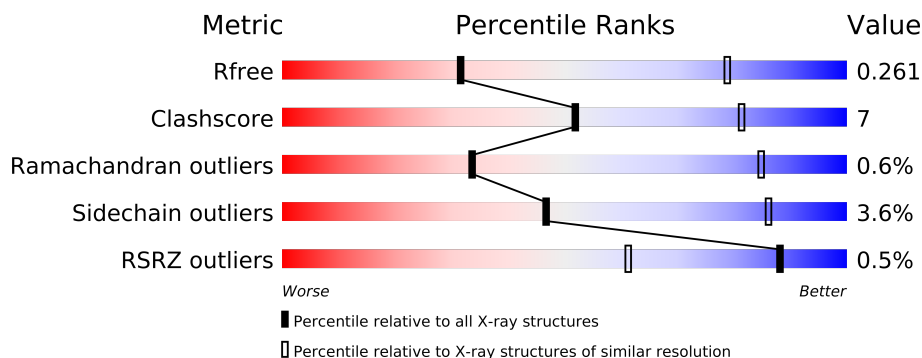
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 3.41 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)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	66092	1013 (3.54-3.30)
Clashscore	79885	1270 (3.54-3.30)
Ramachandran outliers	78287	1232 (3.54-3.30)
Sidechain outliers	78261	1232 (3.54-3.30)
RSRZ outliers	66119	1013 (3.54-3.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	473	
1	B	473	
2	C	221	
2	E	221	
3	D	211	
3	F	211	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
4	BR	A	474	-	X
4	BR	B	474	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13211 atoms, of which 0 are hydrogen and 0 are deuterium.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 H(+)/Cl(-) exchange transporter clcA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	444	Total	C	N	O	S	0	0	0
			3326	2184	560	562	20			
1	B	441	Total	C	N	O	S	0	0	0
			3297	2168	553	556	20			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	445	ALA	TYR	ENGINEERED	UNP P37019
B	445	ALA	TYR	ENGINEERED	UNP P37019

- Molecule 2 is a protein called Fab fragment, Heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	221	Total	C	N	O	S	0	0	0
			1672	1077	274	315	6			
2	E	221	Total	C	N	O	S	0	0	0
			1672	1077	274	315	6			

- Molecule 3 is a protein called Fab fragment, Light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	211	Total	C	N	O	S	0	0	0
			1621	1008	271	334	8			
3	F	211	Total	C	N	O	S	0	0	0
			1621	1008	271	334	8			

- Molecule 4 is BROMIDE ION (three-letter code: BR) (formula: Br).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Br	0	0
			1	1		

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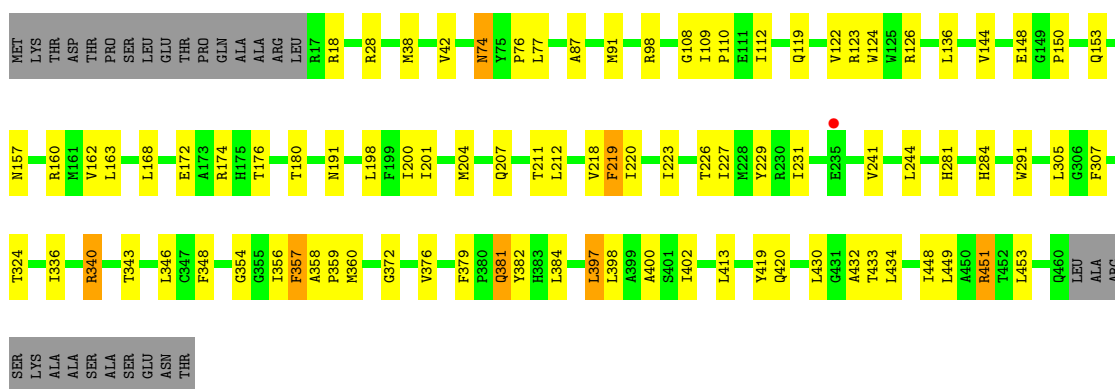
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Br	0	0
			1	1		

### 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 errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). 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.

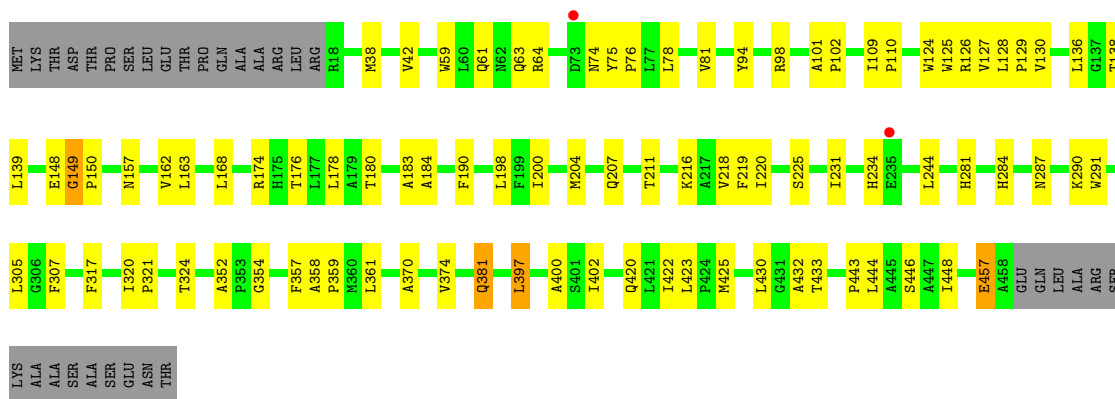
- Molecule 1: H(+)/Cl(-) exchange transporter clcA

Chain A:



- Molecule 1: H(+)/Cl(-) exchange transporter clcA

Chain B:



- Molecule 2: Fab fragment, Heavy chain

Chain C:



- Molecule 2: Fab fragment, Heavy chain

V2	V160	K151	G152	Y153	S164	C203	H207	P208	R221	A222	S30	R31	Y32	W33	M34	S35	M32	P33	P62	K65	L79	Y80	L81	V86	T91	R98	L99	Y107	F108	D109	T115	T118	T125	P126	P127	Y130	P131	L132	A140	L149
E6	K151	G152	Y153	S164	C203	H207	P208	R221	A222	S30	R31	Y32	W33	M34	S35	M32	P33	P62	K65	L79	Y80	L81	V86	T91	R98	L99	Y107	F108	D109	T115	T118	T125	P126	P127	Y130	P131	L132	A140	L149	
G9	K151	G152	Y153	S164	C203	H207	P208	R221	A222	S30	R31	Y32	W33	M34	S35	M32	P33	P62	K65	L79	Y80	L81	V86	T91	R98	L99	Y107	F108	D109	T115	T118	T125	P126	P127	Y130	P131	L132	A140	L149	
V12	K151	G152	Y153	S164	C203	H207	P208	R221	A222	S30	R31	Y32	W33	M34	S35	M32	P33	P62	K65	L79	Y80	L81	V86	T91	R98	L99	Y107	F108	D109	T115	T118	T125	P126	P127	Y130	P131	L132	A140	L149	
G16	K151	G152	Y153	S164	C203	H207	P208	R221	A222	S30	R31	Y32	W33	M34	S35	M32	P33	P62	K65	L79	Y80	L81	V86	T91	R98	L99	Y107	F108	D109	T115	T118	T125	P126	P127	Y130	P131	L132	A140	L149	
V12	K151	G152	Y153	S164	C203	H207	P208	R221	A222	S30	R31	Y32	W33	M34	S35	M32	P33	P62	K65	L79	Y80	L81	V86	T91	R98	L99	Y107	F108	D109	T115	T118	T125	P126	P127	Y130	P131	L132	A140	L149	
G16	K151	G152	Y153	S164	C203	H207	P208	R221	A222	S30	R31	Y32	W33	M34	S35	M32	P33	P62	K65	L79	Y80	L81	V86	T91	R98	L99	Y107	F108	D109	T115	T118	T125	P126	P127	Y130	P131	L132	A140	L149	
V12	K151	G152	Y153	S164	C203	H207	P208	R221	A222	S30	R31	Y32	W33	M34	S35	M32	P33	P62	K65	L79	Y80	L81	V86	T91	R98	L99	Y107	F108	D109	T115	T118	T125	P126	P127	Y130	P131	L132	A140	L149	
G16	K151	G152	Y153	S164	C203	H207	P208	R221	A222	S30	R31	Y32	W33	M34	S35	M32	P33	P62	K65	L79	Y80	L81	V86	T91	R98	L99	Y107	F108	D109	T115	T118	T125	P126	P127	Y130	P131	L132	A140	L149	
V12	K151	G152	Y153	S164	C203	H207	P208	R221	A222	S30	R31	Y32	W33	M34	S35	M32	P33	P62	K65	L79	Y80	L81	V86	T91	R98	L99	Y107	F108	D109	T115	T118	T125	P126	P127	Y130	P131	L132	A140	L149	
G16	K151	G152	Y153	S164	C203	H207	P208	R221	A222	S30	R31	Y32	W33	M34	S35	M32	P33	P62	K65	L79	Y80	L81	V86	T91	R98	L99	Y107	F108	D109	T115	T118	T125	P126	P127	Y130	P131	L132	A140	L149	
V12	K151	G152	Y153	S164	C203	H207	P208	R221	A222	S30	R31	Y32	W33	M34	S35	M32	P33	P62	K65	L79	Y80	L81	V86	T91	R98	L99	Y107	F108	D109	T115	T118	T125	P126	P127	Y130	P131	L132	A140	L149	
G16	K151	G152	Y153	S164	C203	H207	P208	R221	A222	S30	R31	Y32	W33	M34	S35	M32	P33	P62	K65	L79	Y80	L81	V86	T91	R98	L99	Y107	F108	D109	T115	T118	T125	P126	P127	Y130	P131	L132	A140	L149	
V12	K151	G152	Y153																																					

- Chain D: 

D1	I2	T5	Q6	S7	P8	G16	T22	S27	W46	V69	T76	Y86	W90	P94	Q95	S126	K148	H149	D150	E153	W162	M174	M189	S190	Y191	C192	T193	E194	T199	V205	Q211
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- Chain F: 

K146	W147	K148	I149	D150	G151	W162	Y172	S173	M174	L178	N189	Y191	T192	C193	E194	V205	R210	A211	D1	I2	Q6	S7	P8	G16	T22	S27	Y31	H33	W34	K38	T41	I47	T50	R60	T76	D81	T84	Y85	Y86	C87	Q88	Q89	W90	Q95	T96	F97	G98	F117	P118	P119	S120	T125	S126	G127	V131	N136	K141
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## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	232.07Å 98.14Å 171.07Å 90.00° 131.56° 90.00°	Depositor
Resolution (Å)	40.00 – 3.41 19.96 – 3.40	Depositor EDS
% Data completeness (in resolution range)	96.9 (40.00-3.41) 97.0 (19.96-3.40)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.20 (at 3.44Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.266 , 0.276 0.248 , 0.261	Depositor DCC
$R_{free}$ test set	1855 reflections (5.14%)	DCC
Wilson B-factor (Å <sup>2</sup> )	113.4	Xtriage
Anisotropy	0.467	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.25 , 35.6	EDS
Estimated twinning fraction	0.000 for h,-k,-h-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 39582 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	13211	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	101.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.94% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BR

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	0.35	0/3397	0.50	0/4610
1	B	0.35	0/3368	0.49	0/4572
2	C	0.35	0/1721	0.52	0/2355
2	E	0.35	0/1721	0.51	0/2355
3	D	0.34	0/1660	0.49	0/2257
3	F	0.33	0/1660	0.50	0/2257
All	All	0.35	0/13527	0.50	0/18406

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3326	0	3480	62	0
1	B	3297	0	3453	56	0
2	C	1672	0	1654	11	0
2	E	1672	0	1654	20	0
3	D	1621	0	1546	18	0
3	F	1621	0	1546	36	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	1	0	0	2	0
4	B	1	0	0	2	0
All	All	13211	0	13333	190	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 7.

The worst 5 of 190 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:F:7:SER:HB3	3:F:8:PRO:HD3	1.42	0.98
1:A:381:GLN:HE21	1:A:381:GLN:H	0.95	0.91
1:B:381:GLN:HE21	1:B:381:GLN:H	1.15	0.90
1:A:148:GLU:HG2	1:A:357:PHE:HB3	1.63	0.80
1:B:148:GLU:CD	1:B:148:GLU:H	1.85	0.79

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 X-ray entries followed by that with respect to entries of similar resolution. 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	442/473 (93%)	415 (94%)	26 (6%)	1 (0%)	56	94
1	B	439/473 (93%)	408 (93%)	30 (7%)	1 (0%)	56	94
2	C	219/221 (99%)	202 (92%)	16 (7%)	1 (0%)	38	87
2	E	219/221 (99%)	197 (90%)	18 (8%)	4 (2%)	13	64
3	D	209/211 (99%)	187 (90%)	21 (10%)	1 (0%)	38	87
3	F	209/211 (99%)	191 (91%)	16 (8%)	2 (1%)	22	77
All	All	1737/1810 (96%)	1600 (92%)	127 (7%)	10 (1%)	33	85

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	E	65	LYS
2	E	62	PRO
2	E	140	ALA
2	C	62	PRO
3	F	7	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 X-ray entries followed by that with respect to entries of similar resolution. 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	334/357 (94%)	320 (96%)	14 (4%)	40	83
1	B	331/357 (93%)	315 (95%)	16 (5%)	35	80
2	C	181/181 (100%)	175 (97%)	6 (3%)	50	88
2	E	181/181 (100%)	177 (98%)	4 (2%)	64	92
3	D	185/185 (100%)	179 (97%)	6 (3%)	51	89
3	F	185/185 (100%)	181 (98%)	4 (2%)	64	92
All	All	1397/1446 (97%)	1347 (96%)	50 (4%)	47	86

5 of 50 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	357	PHE
1	B	433	THR
3	F	1	ASP
1	B	381	GLN
1	B	402	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 33 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	157	ASN
1	B	277	GLN
3	F	136	ASN
1	B	207	GLN
1	B	234	HIS

### 5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

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.

### 5.7 Other polymers ⓘ

There are no such residues in this entry.

### 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å <sup>2</sup> )	Q<0.9
1	A	444/473 (93%)	-0.17	1 (0%)	93 77	40, 96, 146, 200	0
1	B	441/473 (93%)	-0.18	2 (0%)	88 61	44, 97, 154, 200	0
2	C	221/221 (100%)	-0.07	2 (0%)	81 47	53, 90, 146, 197	0
2	E	221/221 (100%)	-0.02	0	100 100	48, 99, 157, 200	0
3	D	211/211 (100%)	-0.01	1 (0%)	88 61	48, 109, 157, 179	0
3	F	211/211 (100%)	-0.02	2 (0%)	81 47	40, 89, 147, 181	0
All	All	1749/1810 (96%)	-0.10	8 (0%)	88 61	40, 97, 154, 200	0

The worst 5 of 8 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	73	ASP	3.6
1	A	235	GLU	3.0
2	C	139	ALA	2.7
1	B	235	GLU	2.4
2	C	137	ALA	2.2

### 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

### 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
4	BR	A	474	1/1	0.65	12.81	56,56,56,56	0
4	BR	B	474	1/1	0.57	9.55	56,56,56,56	0

## 6.5 Other polymers

There are no such residues in this entry.