



Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 08:12 am BST

PDB ID : 5TRX
Title : Room temperature structure of an extradiol ring-cleaving dioxygenase from *B.fuscum* determined using serial femtosecond crystallography
Authors : Kovaleva, E.G.; Oberthuer, D.; Tolstikova, A.; Mariani, V.
Deposited on : 2016-10-27
Resolution : 2.38 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

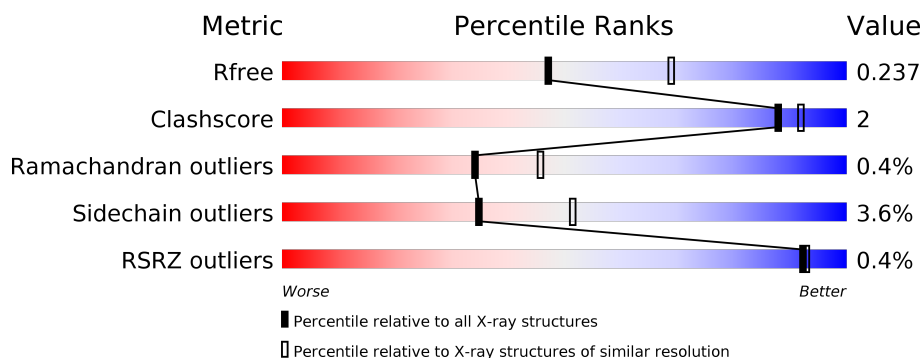
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.38 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}	130704	5509 (2.40-2.36)
Clashscore	141614	6082 (2.40-2.36)
Ramachandran outliers	138981	5973 (2.40-2.36)
Sidechain outliers	138945	5975 (2.40-2.36)
RSRZ outliers	127900	5397 (2.40-2.36)

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 ≥ 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	365	<div> <div style="width: 92%;"></div> <div style="width: 5%;"></div> <div style="width: 3%;"></div> <div style="width: 2%;"></div> <div style="width: 2%;"></div> </div> 92% 5% . .
1	B	365	<div> <div style="width: 92%;"></div> <div style="width: 6%;"></div> <div style="width: 2%;"></div> <div style="width: 2%;"></div> </div> 92% 6% . .
1	C	365	<div> <div style="width: 86%;"></div> <div style="width: 12%;"></div> <div style="width: 2%;"></div> </div> 86% 12% . .
1	D	365	<div> <div style="width: 90%;"></div> <div style="width: 8%;"></div> <div style="width: 2%;"></div> </div> 90% 8% . .

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 12065 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Homoprotocatechuate 2,3-dioxygenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	358	Total	C	N	O	S	0	0	0
			2896	1827	509	553	7			
1	B	359	Total	C	N	O	S	0	1	0
			2908	1834	511	555	8			
1	C	358	Total	C	N	O	S	0	1	0
			2905	1832	510	556	7			
1	D	359	Total	C	N	O	S	0	1	0
			2908	1834	511	555	8			

- Molecule 2 is FE (II) ION (three-letter code: FE2) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Fe	0	0
			1	1		
2	A	1	Total	Fe	0	0
			1	1		
2	D	1	Total	Fe	0	0
			1	1		
2	C	1	Total	Fe	0	0
			1	1		

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Cl	0	0
			1	1		
3	A	1	Total	Cl	0	0
			1	1		
3	D	1	Total	Cl	0	0
			1	1		
3	C	1	Total	Cl	0	0
			1	1		

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	111	Total 111	O 111	0	0
5	B	134	Total 134	O 134	0	1
5	C	101	Total 101	O 101	0	0
5	D	93	Total 93	O 93	0	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 the various outlier classes 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: Homoprotocatechuate 2,3-dioxygenase

Chain A: 




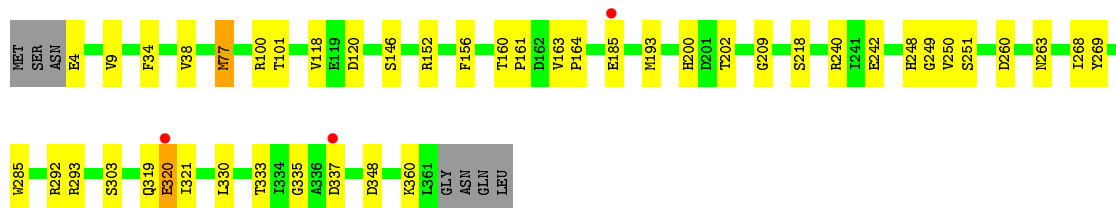
- Molecule 1: Homoprotocatechuate 2,3-dioxygenase

Chain B: 




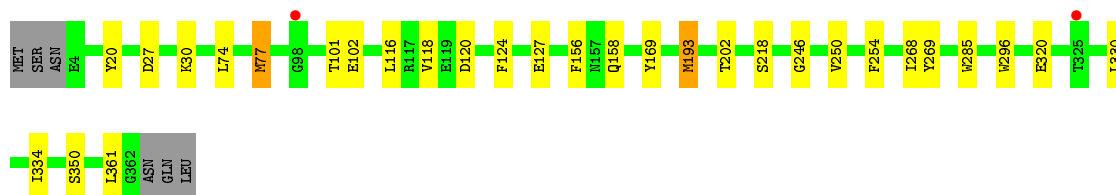
- Molecule 1: Homoprotocatechuate 2,3-dioxygenase

Chain C: 



- Molecule 1: Homoprotocatechuate 2,3-dioxygenase

Chain D: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 ₁ 2 ₁ 2	Depositor
Cell constants a, b, c, α , β , γ	111.57Å 154.86Å 101.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.38 19.96 – 2.38	Depositor EDS
% Data completeness (in resolution range)	99.7 (20.00-2.38) 99.9 (19.96-2.38)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.44 (at 2.38Å)	Xtriage
Refinement program	REFMAC 5.8.0069	Depositor
R, R_{free}	0.184 , 0.232 0.192 , 0.237	Depositor DCC
R_{free} test set	3568 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	41.0	Xtriage
Anisotropy	0.212	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 42.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	12065	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.43% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CA, FE2, CL

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	0.58	0/2972	0.76	0/4036
1	B	0.58	0/2984	0.75	1/4051 (0.0%)
1	C	0.55	0/2981	0.71	1/4048 (0.0%)
1	D	0.56	0/2984	0.72	0/4051
All	All	0.57	0/11921	0.74	2/16186 (0.0%)

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	2
1	B	0	1
1	C	0	4
1	D	0	1
All	All	0	8

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	152	ARG	NE-CZ-NH1	5.35	122.97	120.30
1	B	239	ASP	CB-CG-OD1	5.09	122.88	118.30

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	118	VAL	Peptide
1	A	248	HIS	Peptide
1	B	268	ILE	Peptide
1	C	209	GLY	Peptide
1	C	268	ILE	Peptide
1	C	319	GLN	Peptide
1	C	335	GLY	Peptide
1	D	268	ILE	Peptide

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	2896	0	2748	8	0
1	B	2908	0	2759	8	0
1	C	2905	0	2753	15	0
1	D	2908	0	2759	16	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	1	0
3	D	1	0	0	0	0
4	B	1	0	0	0	0
5	A	111	0	0	0	0
5	B	134	0	0	0	0
5	C	101	0	0	0	0
5	D	93	0	0	0	0
All	All	12065	0	11019	46	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 2.

All (46) 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:D:101:THR:HG22	1:D:118:VAL:HG12	1.58	0.85
1:D:101:THR:HG22	1:D:118:VAL:CG1	2.33	0.58
1:B:226:ILE:HD12	1:D:254:PHE:CE1	2.40	0.56
1:C:293:ARG:HB3	3:C:402:CL:CL	2.44	0.55
1:B:334:ILE:HD12	1:B:361:LEU:HD21	1.90	0.54
1:B:218:SER:HA	1:B:269:TYR:O	2.07	0.54
1:A:101:THR:HB	1:A:116:LEU:HD11	1.92	0.52
1:D:320:GLU:CD	1:D:320:GLU:H	2.14	0.50
1:C:330:LEU:C	1:C:330:LEU:HD23	2.32	0.50
1:A:334:ILE:HG13	1:A:361:LEU:HD21	1.94	0.50
1:C:218:SER:HA	1:C:269:TYR:O	2.12	0.49
1:D:74:LEU:HD21	1:D:77[A]:MET:HG2	1.95	0.49
1:C:101:THR:HG22	1:C:118:VAL:HG12	1.93	0.48
1:D:101:THR:HB	1:D:116:LEU:HD11	1.95	0.48
1:D:334:ILE:HD12	1:D:361:LEU:HD21	1.94	0.48
1:C:250:VAL:HG22	1:C:285:TRP:CD1	2.48	0.48
1:B:139:HIS:CD2	1:B:140:MET:HG3	2.49	0.47
1:A:102:GLU:OE2	1:A:104:ARG:NE	2.48	0.47
1:C:156:PHE:O	1:C:202:THR:HA	2.15	0.46
1:D:250:VAL:HG22	1:D:285:TRP:CD1	2.50	0.46
1:D:77[A]:MET:HE3	1:D:156:PHE:CD2	2.52	0.45
1:B:74:LEU:HD13	1:B:212:LEU:HD22	1.99	0.44
1:C:240:ARG:HH22	1:C:263:ASN:ND2	2.15	0.44
1:C:160:THR:OG1	1:C:161:PRO:HD2	2.17	0.44
1:D:218:SER:HA	1:D:269:TYR:O	2.18	0.44
1:B:260:ASP:C	1:B:260:ASP:OD1	2.57	0.43
1:D:330:LEU:C	1:D:330:LEU:HD23	2.38	0.43
1:C:163:VAL:N	1:C:164:PRO:CD	2.81	0.43
1:D:246:GLY:HA2	1:D:296:TRP:CZ3	2.53	0.43
1:A:192:TRP:CE2	1:A:250:VAL:HG11	2.54	0.43
1:A:86:ASP:HA	1:A:89:LYS:HB2	2.00	0.42
1:C:34:PHE:O	1:C:38:VAL:HB	2.19	0.42
1:A:200:HIS:HD2	1:A:203:ALA:HB2	1.84	0.42
1:D:20:TYR:OH	1:D:127:GLU:OE2	2.36	0.42
1:D:193:MET:HG2	1:D:202:THR:O	2.19	0.42
1:C:292:ARG:NH2	1:C:333:THR:HG21	2.34	0.42
1:D:27:ASP:C	1:D:27:ASP:OD1	2.57	0.42
1:D:124:PHE:CZ	1:D:158:GLN:HB3	2.54	0.41
1:A:183:ASP:OD1	1:A:183:ASP:C	2.59	0.41
1:C:260:ASP:OD1	1:C:260:ASP:C	2.59	0.41
1:B:60:ILE:HB	1:B:132:THR:HG21	2.02	0.41
1:C:77:MET:HE3	1:C:156:PHE:CG	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:143:ASP:OD1	1:B:143:ASP:N	2.53	0.40
1:A:120:ASP:C	1:A:120:ASP:OD1	2.59	0.40
1:C:248:HIS:HA	1:C:293:ARG:O	2.21	0.40
1:C:242:GLU:OE2	1:C:303:SER:OG	2.38	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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	356/365 (98%)	339 (95%)	16 (4%)	1 (0%)	41	53
1	B	358/365 (98%)	343 (96%)	14 (4%)	1 (0%)	41	53
1	C	357/365 (98%)	341 (96%)	13 (4%)	3 (1%)	19	27
1	D	358/365 (98%)	345 (96%)	13 (4%)	0	100	100
All	All	1429/1460 (98%)	1368 (96%)	56 (4%)	5 (0%)	34	53

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	320	GLU
1	A	249	GLY
1	C	251	SER
1	B	271	GLN
1	C	249	GLY

5.3.2 Protein sidechains [i](#)

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	307/313 (98%)	294 (96%)	13 (4%)	30	44
1	B	308/313 (98%)	298 (97%)	10 (3%)	39	56
1	C	308/313 (98%)	294 (96%)	14 (4%)	27	41
1	D	308/313 (98%)	300 (97%)	8 (3%)	46	64
All	All	1231/1252 (98%)	1186 (96%)	45 (4%)	35	50

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	VAL
1	A	77	MET
1	A	89	LYS
1	A	102	GLU
1	A	104	ARG
1	A	118	VAL
1	A	120	ASP
1	A	168	LYS
1	A	193	MET
1	A	200	HIS
1	A	260	ASP
1	A	328	SER
1	A	360	LYS
1	B	100	ARG
1	B	102	GLU
1	B	105	LYS
1	B	120	ASP
1	B	176	ARG
1	B	193	MET
1	B	260	ASP
1	B	310	LYS
1	B	331	GLU
1	B	361	LEU
1	C	4	GLU
1	C	9	VAL
1	C	77	MET
1	C	100	ARG
1	C	120	ASP
1	C	146	SER
1	C	185	GLU

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Mol	Chain	Res	Type
1	C	193	MET
1	C	200	HIS
1	C	320	GLU
1	C	321	ILE
1	C	337	ASP
1	C	348	ASP
1	C	360	LYS
1	D	30	LYS
1	D	77[A]	MET
1	D	77[B]	MET
1	D	102	GLU
1	D	120	ASP
1	D	169	TYR
1	D	193	MET
1	D	350	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	263	ASN

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](#)

Of 9 ligands modelled in this entry, 9 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.

No monomer is involved in short contacts.

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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, 95th 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 ²)	Q<0.9
1	A	358/365 (98%)	-0.48	0	100 100	30, 40, 57, 83	0
1	B	359/365 (98%)	-0.50	1 (0%)	94 94	29, 39, 56, 75	0
1	C	358/365 (98%)	-0.33	3 (0%)	86 86	32, 45, 65, 87	0
1	D	359/365 (98%)	-0.36	2 (0%)	89 89	32, 44, 63, 81	0
All	All	1434/1460 (98%)	-0.42	6 (0%)	92 93	29, 42, 60, 87	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	325	THR	4.0
1	C	185	GLU	3.0
1	D	98	GLY	2.6
1	C	337	ASP	2.5
1	C	320	GLU	2.4
1	B	48	GLU	2.1

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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. The B-factors column lists the minimum,

median, 95th 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	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	FE2	A	401	1/1	0.98	0.09	39,39,39,39	0
2	FE2	C	401	1/1	0.98	0.07	45,45,45,45	0
2	FE2	D	401	1/1	0.99	0.07	44,44,44,44	0
3	CL	A	402	1/1	0.99	0.12	36,36,36,36	0
2	FE2	B	401	1/1	0.99	0.09	40,40,40,40	0
4	CA	B	402	1/1	0.99	0.05	48,48,48,48	0
3	CL	B	403	1/1	0.99	0.08	35,35,35,35	0
3	CL	C	402	1/1	0.99	0.03	36,36,36,36	0
3	CL	D	402	1/1	0.99	0.10	36,36,36,36	0

6.5 Other polymers

There are no such residues in this entry.