



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 12:24 AM UTC

PDB ID : 6TPI / pdb_00006tpi
Title : EnvC bound to the FtsX periplasmic domain
Authors : Crow, A.
Deposited on : 2019-12-13
Resolution : 2.10 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

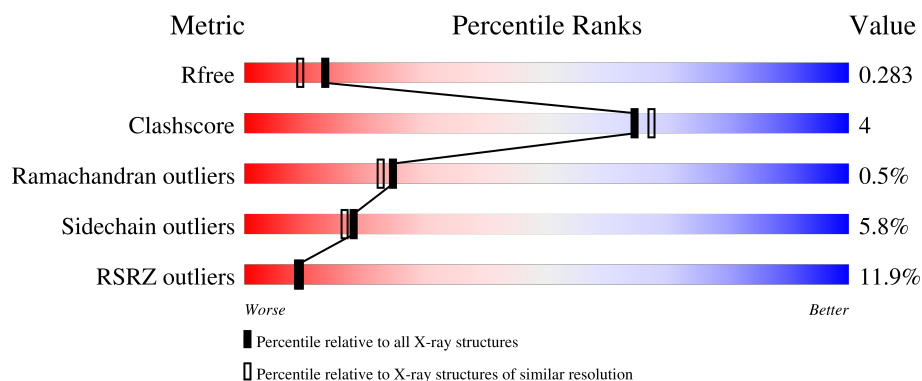
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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 of 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	386	5% 88% 10% ..
2	B	110	% 85% 5% 8%
2	C	110	43% 65% 19% • 12%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4767 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 Murein hydrolase activator EnvC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	380	Total	C	N	O	S	0	4	0
			3012	1840	586	581	5			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	34	MET	-	initiating methionine	UNP P37690

- Molecule 2 is a protein called Cell division protein FtsX.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	101	Total	C	N	O	S	0	0	0
			776	482	132	160	2			
2	C	97	Total	C	N	O	S	0	0	0
			750	469	128	151	2			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	108	MET	-	initiating methionine	UNP P0AC30
B	109	GLY	-	expression tag	UNP P0AC30
B	210	LEU	-	expression tag	UNP P0AC30
B	211	GLU	-	expression tag	UNP P0AC30
B	212	HIS	-	expression tag	UNP P0AC30
B	213	HIS	-	expression tag	UNP P0AC30
B	214	HIS	-	expression tag	UNP P0AC30
B	215	HIS	-	expression tag	UNP P0AC30
B	216	HIS	-	expression tag	UNP P0AC30
B	217	HIS	-	expression tag	UNP P0AC30
C	108	MET	-	initiating methionine	UNP P0AC30
C	109	GLY	-	expression tag	UNP P0AC30
C	210	LEU	-	expression tag	UNP P0AC30

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Chain	Residue	Modelled	Actual	Comment	Reference
C	211	GLU	-	expression tag	UNP P0AC30
C	212	HIS	-	expression tag	UNP P0AC30
C	213	HIS	-	expression tag	UNP P0AC30
C	214	HIS	-	expression tag	UNP P0AC30
C	215	HIS	-	expression tag	UNP P0AC30
C	216	HIS	-	expression tag	UNP P0AC30
C	217	HIS	-	expression tag	UNP P0AC30

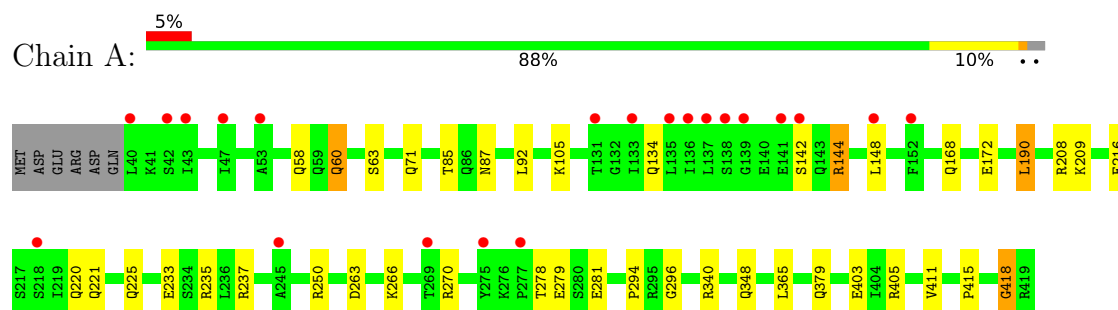
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	173	Total 173	O 173	0	0
3	B	53	Total 53	O 53	0	0
3	C	3	Total 3	O 3	0	0

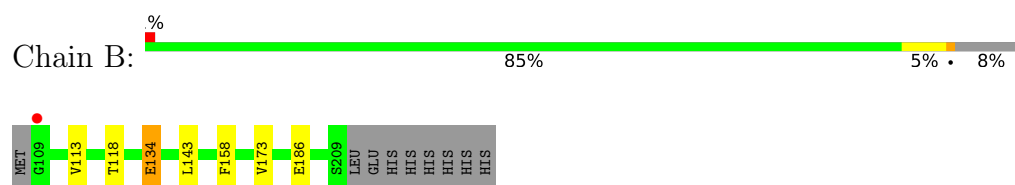
3 Residue-property plots [i](#)

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 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.

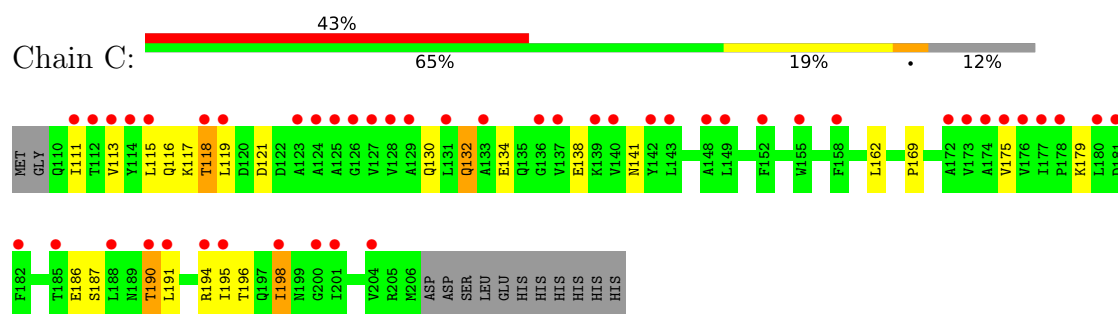
- Molecule 1: Murein hydrolase activator EnvC



- Molecule 2: Cell division protein FtsX



- Molecule 2: Cell division protein FtsX



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	67.03Å 100.47Å 107.78Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	55.82 – 2.10 55.82 – 2.10	Depositor EDS
% Data completeness (in resolution range)	100.0 (55.82-2.10) 100.0 (55.82-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.20 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.215 , 0.275 0.225 , 0.283	Depositor DCC
R_{free} test set	2102 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å ²)	38.3	Xtriage
Anisotropy	0.183	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 30.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	4767	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.49% 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](#)

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	1.02	1/3043 (0.0%)	1.51	3/4079 (0.1%)
2	B	1.02	0/785	1.49	2/1064 (0.2%)
2	C	1.07	0/759	1.47	0/1029
All	All	1.03	1/4587 (0.0%)	1.50	5/6172 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	411	VAL	C-O	5.10	1.29	1.23

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	379	GLN	CB-CA-C	5.67	119.89	109.46
1	A	144	ARG	CA-C-N	5.60	126.20	119.98
1	A	144	ARG	C-N-CA	5.60	126.20	119.98
2	B	158	PHE	CA-CB-CG	5.12	118.92	113.80
2	B	118	THR	CA-CB-OG1	-5.11	101.93	109.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	3012	0	3042	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	776	0	755	3	0
2	C	750	0	739	13	0
3	A	173	0	0	3	0
3	B	53	0	0	0	0
3	C	3	0	0	0	0
All	All	4767	0	4536	35	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.

All (35) 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)
2:C:132:GLN:HE21	2:C:132:GLN:HA	1.38	0.89
1:A:233[B]:GLU:OE1	1:A:237[B]:ARG:NH1	2.26	0.68
1:A:418:GLY:HA2	3:A:538:HOH:O	1.95	0.66
1:A:60:GLN:HE21	1:A:60:GLN:HA	1.67	0.59
1:A:365:LEU:C	1:A:365:LEU:HD23	2.29	0.57
1:A:233[A]:GLU:O	1:A:237[A]:ARG:HG3	2.05	0.56
2:C:162:LEU:HD22	2:C:169:PRO:HG2	1.87	0.56
1:A:85:THR:HG23	1:A:190:LEU:CD2	2.40	0.52
1:A:365:LEU:HB3	1:A:403:GLU:HB2	1.92	0.51
1:A:296:GLY:O	1:A:418:GLY:HA3	2.11	0.50
2:C:138:GLU:HG2	2:C:179:LYS:HA	1.93	0.50
2:B:143:LEU:HB2	2:B:173:VAL:HG13	1.93	0.50
1:A:237[B]:ARG:NH2	3:A:515:HOH:O	2.45	0.50
2:C:195:ILE:O	2:C:198:ILE:HG23	2.11	0.50
1:A:85:THR:HG23	1:A:190:LEU:HD22	1.92	0.49
1:A:278:THR:OG1	1:A:281:GLU:HG3	2.12	0.49
2:C:130:GLN:CD	2:C:198:ILE:HD12	2.37	0.49
2:C:162:LEU:HD22	2:C:169:PRO:CG	2.42	0.49
2:C:187:SER:O	2:C:190:THR:HG22	2.15	0.46
1:A:250:ARG:CZ	1:A:340:ARG:HD2	2.46	0.45
2:C:191:LEU:HA	2:C:194:ARG:HD2	1.98	0.45
2:C:111:ILE:HD11	2:C:191:LEU:HD12	1.98	0.44
1:A:168:GLN:HE21	1:A:172:GLU:HG3	1.82	0.44
2:C:141:ASN:HB3	2:C:175:VAL:HG12	1.99	0.44
1:A:71:GLN:OE1	1:A:208:ARG:HA	2.19	0.42
1:A:220:GLN:O	1:A:225:GLN:NE2	2.36	0.42
1:A:235:ARG:HH21	1:A:348:GLN:HB3	1.83	0.41
2:B:186:GLU:OE1	2:B:186:GLU:HA	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:175:VAL:O	2:C:175:VAL:HG13	2.20	0.41
1:A:294:PRO:HB2	1:A:415:PRO:HB2	2.03	0.41
1:A:263:ASP:O	1:A:266:LYS:N	2.41	0.41
2:C:115:LEU:HD12	2:C:115:LEU:N	2.36	0.41
1:A:405:ARG:NH2	3:A:520:HOH:O	2.47	0.40
2:C:116:GLN:HB3	2:C:118:THR:HG22	2.03	0.40
2:B:134:GLU:OE1	2:B:134:GLU:HA	2.21	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	382/386 (99%)	369 (97%)	10 (3%)	3 (1%)	16	12
2	B	99/110 (90%)	97 (98%)	2 (2%)	0	100	100
2	C	95/110 (86%)	93 (98%)	2 (2%)	0	100	100
All	All	576/606 (95%)	559 (97%)	14 (2%)	3 (0%)	24	22

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	134	GLN
1	A	142	SER
1	A	418	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	305/307 (99%)	291 (95%)	14 (5%)	24	25
2	B	83/92 (90%)	81 (98%)	2 (2%)	43	49
2	C	80/92 (87%)	69 (86%)	11 (14%)	3	2
All	All	468/491 (95%)	441 (94%)	27 (6%)	18	16

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	58	GLN
1	A	60	GLN
1	A	63	SER
1	A	87	ASN
1	A	92	LEU
1	A	105	LYS
1	A	144	ARG
1	A	148	LEU
1	A	190	LEU
1	A	209	LYS
1	A	216	GLU
1	A	221	GLN
1	A	270	ARG
1	A	279	GLU
2	B	113	VAL
2	B	134	GLU
2	C	113	VAL
2	C	117	LYS
2	C	118	THR
2	C	119	LEU
2	C	121	ASP
2	C	132	GLN
2	C	134	GLU
2	C	186	GLU
2	C	190	THR
2	C	196	THR
2	C	198	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	GLN
1	A	109	GLN
1	A	113	GLN
1	A	143	GLN
1	A	149	GLN
1	A	168	GLN
1	A	194	GLN
1	A	369	ASN
1	A	370	GLN
2	B	141	ASN
2	B	154	ASN
2	C	132	GLN
2	C	154	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 oligosaccharides 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.

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, 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	380/386 (98%)	0.27	21 (5%) 30 32	17, 45, 103, 142	4 (1%)
2	B	101/110 (91%)	0.17	1 (0%) 79 81	35, 48, 72, 103	0
2	C	97/110 (88%)	2.12	47 (48%) 0 0	55, 124, 166, 194	0
All	All	578/606 (95%)	0.56	69 (11%) 9 9	17, 50, 141, 194	4 (0%)

All (69) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	195	ILE	5.8
2	C	198	ILE	5.4
1	A	136	ILE	5.2
2	C	131	LEU	5.1
2	C	113	VAL	5.1
2	C	177	ILE	5.0
1	A	137	LEU	4.7
2	C	128	VAL	4.7
2	C	127	VAL	4.2
2	C	137	VAL	4.2
2	C	174	ALA	4.2
2	C	115	LEU	4.1
2	C	188	LEU	4.0
2	C	175	VAL	4.0
2	C	204	VAL	4.0
1	A	135	LEU	3.9
2	C	129	ALA	3.9
1	A	131	THR	3.8
2	C	173	VAL	3.7
1	A	133	ILE	3.7
2	C	191	LEU	3.6
2	C	142	TYR	3.6
1	A	43	ILE	3.6

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Mol	Chain	Res	Type	RSRZ
2	C	176	VAL	3.5
2	C	125	ALA	3.4
2	C	124	ALA	3.4
2	C	200	GLY	3.4
2	C	111	ILE	3.3
2	C	143	LEU	3.2
2	C	178	PRO	3.2
1	A	269	THR	3.1
2	C	133	ALA	3.1
1	A	47	ILE	3.1
1	A	40	LEU	3.0
1	A	275	TYR	3.0
2	C	119	LEU	2.8
1	A	152	PHE	2.8
2	C	182	PHE	2.8
2	C	201	ILE	2.8
2	B	109	GLY	2.8
2	C	123	ALA	2.8
2	C	185	THR	2.8
2	C	112	THR	2.7
1	A	142	SER	2.7
2	C	149	LEU	2.6
1	A	53	ALA	2.6
2	C	180	LEU	2.6
2	C	158	PHE	2.6
2	C	126	GLY	2.6
2	C	152	PHE	2.5
1	A	139	GLY	2.5
1	A	245	ALA	2.4
1	A	148	LEU	2.4
1	A	277	PRO	2.4
2	C	114	TYR	2.3
2	C	140	VAL	2.3
2	C	172	ALA	2.3
2	C	139	LYS	2.3
2	C	118	THR	2.3
2	C	136	GLY	2.3
1	A	138	SER	2.2
2	C	194	ARG	2.2
2	C	181	ASP	2.2
1	A	141	GLU	2.1
1	A	42	SER	2.1

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Mol	Chain	Res	Type	RSRZ
2	C	190	THR	2.1
1	A	218	SER	2.0
2	C	148	ALA	2.0
2	C	155	TRP	2.0

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 oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.