



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 10:45 AM UTC

PDB ID : 6WWD / pdb_00006wwd
Title : Crystal structure of Nucleoside-triphosphatase / dITP/XTP pyrophosphatase from Mycobacterium abscessus ATCC 19977 / DSM 44196
Authors : Seattle Structural Genomics Center for Infectious Disease (SSGCID)
Deposited on : 2020-05-09
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

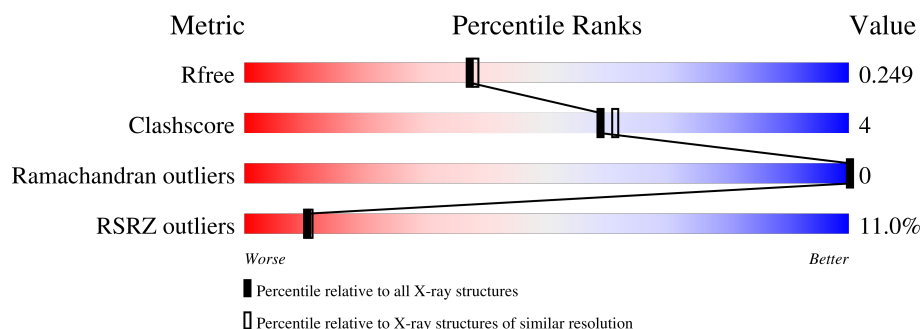
1 Overall quality at a glance

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)
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	213	8% 85% 8% 8%
1	B	213	8% 79% 10% 11%
1	C	213	14% 80% 10% 10%
1	D	213	9% 85% 8% 7%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6140 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 dITP/XTP pyrophosphatase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	196	Total	C	N	O	S	0	6	0
			1428	892	256	274	6			
1	B	190	Total	C	N	O	S	0	4	0
			1383	870	248	259	6			
1	C	191	Total	C	N	O	S	0	3	0
			1354	850	242	259	3			
1	D	199	Total	C	N	O	S	0	1	0
			1425	891	250	279	5			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	207	GLY	-	expression tag	UNP B1MLZ4
A	208	HIS	-	expression tag	UNP B1MLZ4
A	209	HIS	-	expression tag	UNP B1MLZ4
A	210	HIS	-	expression tag	UNP B1MLZ4
A	211	HIS	-	expression tag	UNP B1MLZ4
A	212	HIS	-	expression tag	UNP B1MLZ4
A	213	HIS	-	expression tag	UNP B1MLZ4
B	207	GLY	-	expression tag	UNP B1MLZ4
B	208	HIS	-	expression tag	UNP B1MLZ4
B	209	HIS	-	expression tag	UNP B1MLZ4
B	210	HIS	-	expression tag	UNP B1MLZ4
B	211	HIS	-	expression tag	UNP B1MLZ4
B	212	HIS	-	expression tag	UNP B1MLZ4
B	213	HIS	-	expression tag	UNP B1MLZ4
C	207	GLY	-	expression tag	UNP B1MLZ4
C	208	HIS	-	expression tag	UNP B1MLZ4
C	209	HIS	-	expression tag	UNP B1MLZ4
C	210	HIS	-	expression tag	UNP B1MLZ4
C	211	HIS	-	expression tag	UNP B1MLZ4
C	212	HIS	-	expression tag	UNP B1MLZ4
C	213	HIS	-	expression tag	UNP B1MLZ4

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Chain	Residue	Modelled	Actual	Comment	Reference
D	207	GLY	-	expression tag	UNP B1MLZ4
D	208	HIS	-	expression tag	UNP B1MLZ4
D	209	HIS	-	expression tag	UNP B1MLZ4
D	210	HIS	-	expression tag	UNP B1MLZ4
D	211	HIS	-	expression tag	UNP B1MLZ4
D	212	HIS	-	expression tag	UNP B1MLZ4
D	213	HIS	-	expression tag	UNP B1MLZ4

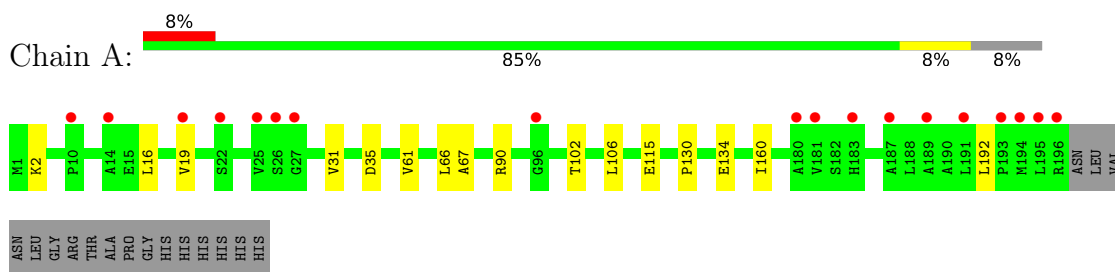
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	128	Total 130	O 130	0	3
2	B	134	Total 136	O 136	0	2
2	C	125	Total 125	O 125	0	1
2	D	158	Total 159	O 159	0	1

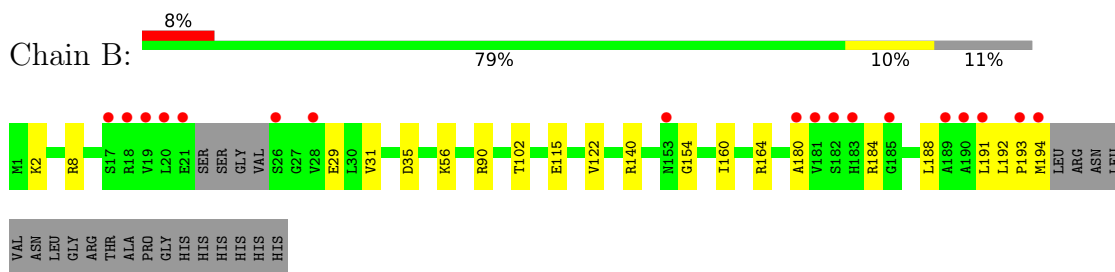
3 Residue-property plots [i](#)

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.

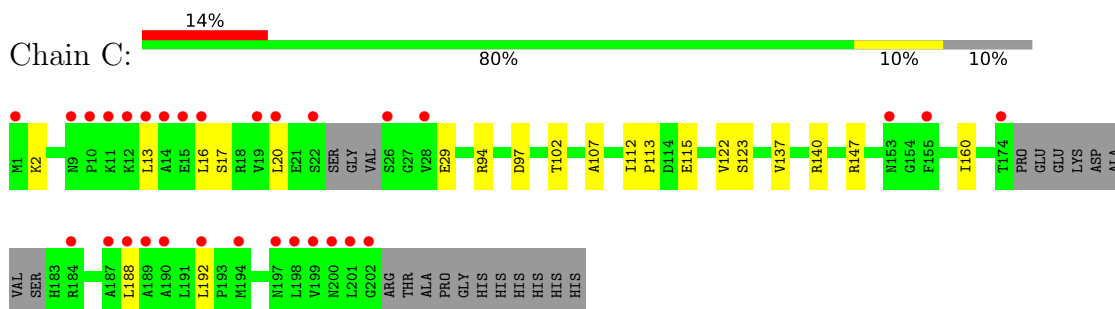
- Molecule 1: dITP/XTP pyrophosphatase



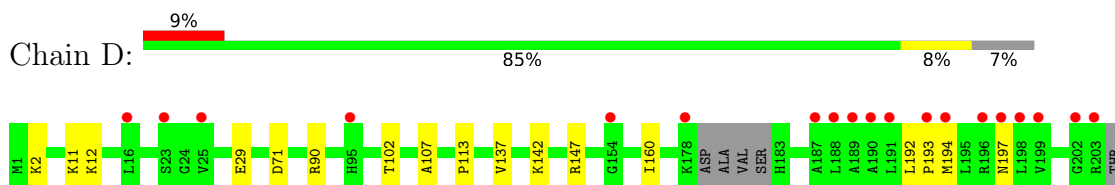
- Molecule 1: dITP/XTP pyrophosphatase



- Molecule 1: dITP/XTP pyrophosphatase



- Molecule 1: dITP/XTP pyrophosphatase



ALA
PRO
GLY
HIS
HIS
HIS
HIS
HIS
HIS

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	50.69Å 104.04Å 146.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.90 – 2.10 47.90 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.0 (47.90-2.10) 99.1 (47.90-2.10)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.06 (at 2.10Å)	Xtriage
Refinement program	PHENIX 1.18	Depositor
R, R_{free}	0.186 , 0.244 0.194 , 0.249	Depositor DCC
R_{free} test set	1963 reflections (4.26%)	wwPDB-VP
Wilson B-factor (Å ²)	19.8	Xtriage
Anisotropy	0.331	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 58.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6140	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 24.21 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.0040e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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	0.33	0/1470	0.54	0/2003
1	B	0.31	0/1417	0.54	0/1927
1	C	0.31	0/1384	0.50	0/1888
1	D	0.33	0/1450	0.54	0/1975
All	All	0.32	0/5721	0.53	0/7793

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 [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	1428	0	1407	14	0
1	B	1383	0	1388	15	0
1	C	1354	0	1296	14	0
1	D	1425	0	1389	16	0
2	A	130	0	0	0	0
2	B	136	0	0	4	0
2	C	125	0	0	1	0
2	D	159	0	0	3	0
All	All	6140	0	5480	49	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 (49) 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:164:ARG:NH1	2:B:304:HOH:O	2.28	0.66
1:B:8:ARG:NH1	2:B:305:HOH:O	2.29	0.64
1:D:113:PRO:HA	1:D:147:ARG:HH22	1.63	0.64
1:A:19:VAL:HG21	1:D:197:ASN:HB2	1.79	0.62
1:C:102:THR:HG23	1:C:160:ILE:HD13	1.82	0.62
1:A:102[B]:THR:HG23	1:A:160:ILE:HD13	1.80	0.61
1:D:2:LYS:HG2	1:D:29:GLU:HG3	1.81	0.61
1:C:97:ASP:OD1	2:C:301:HOH:O	2.16	0.60
1:A:16:LEU:HB3	1:D:194:MET:HE3	1.86	0.57
1:A:192:LEU:HD21	1:D:137[B]:VAL:HG23	1.86	0.56
1:C:13:LEU:O	1:C:17:SER:OG	2.25	0.55
1:B:90[A]:ARG:NH2	1:D:107:ALA:O	2.41	0.53
1:D:147:ARG:NH1	2:D:301:HOH:O	2.35	0.53
1:C:113:PRO:HA	1:C:147:ARG:NH2	2.24	0.53
1:C:115:GLU:H	1:C:115:GLU:CD	2.18	0.52
1:C:188:LEU:O	1:C:192:LEU:HG	2.11	0.51
1:A:16:LEU:HD13	1:D:194:MET:HE2	1.94	0.50
1:A:90[B]:ARG:NH2	1:C:107:ALA:O	2.43	0.50
1:D:102:THR:HG23	1:D:160:ILE:HD13	1.94	0.50
1:B:192:LEU:HD21	1:C:137[B]:VAL:HG23	1.95	0.48
1:A:115:GLU:H	1:A:115:GLU:CD	2.22	0.47
1:C:94:ARG:NH2	1:C:97:ASP:OD2	2.48	0.47
1:A:19:VAL:HG21	1:D:197:ASN:CB	2.43	0.47
1:A:31:VAL:HG13	1:A:35:ASP:HB2	1.96	0.47
1:C:16:LEU:O	1:C:20:LEU:HG	2.16	0.46
1:C:122:VAL:HG22	1:C:140:ARG:HG2	1.97	0.46
1:D:29:GLU:HG2	2:D:314:HOH:O	2.16	0.46
1:C:2:LYS:HA	1:C:29:GLU:O	2.16	0.46
1:B:31:VAL:HG23	1:B:35:ASP:HB2	1.98	0.45
1:B:154:GLY:O	2:B:301:HOH:O	2.20	0.45
1:D:12:LYS:HD3	1:D:71:ASP:OD2	2.17	0.45
1:B:122:VAL:HG22	1:B:140:ARG:HG2	1.99	0.45
1:A:2:LYS:HB2	1:A:66:LEU:HD22	2.00	0.44
1:B:194:MET:HE3	1:B:194:MET:HB3	1.78	0.43
1:D:90:ARG:HG2	2:D:398:HOH:O	2.18	0.43
1:B:56:LYS:HG2	2:B:421:HOH:O	2.19	0.43
1:B:188:LEU:HA	1:B:191:LEU:HD12	2.00	0.43
1:B:180:ALA:HB1	1:B:184:ARG:HH12	1.84	0.43
1:D:11:LYS:HA	1:D:11:LYS:HD3	1.80	0.43
1:A:61:VAL:HG22	1:A:66:LEU:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2:LYS:HA	1:B:29:GLU:O	2.19	0.42
1:A:134:GLU:HB2	1:D:142:LYS:HB2	2.01	0.42
1:B:115:GLU:H	1:B:115:GLU:CD	2.27	0.42
1:B:102:THR:HG23	1:B:160:ILE:HD13	2.02	0.41
1:B:193:PRO:HD2	1:C:123:SER:OG	2.21	0.41
1:D:192:LEU:HB2	1:D:193:PRO:HD3	2.02	0.41
1:A:67:ALA:HB2	1:A:130:PRO:HD3	2.03	0.41
1:A:106:LEU:HA	1:A:106:LEU:HD23	1.83	0.41
1:C:112:ILE:O	1:C:147:ARG:NH2	2.53	0.41

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	168/213 (79%)	166 (99%)	2 (1%)	0	100	100
1	B	181/213 (85%)	178 (98%)	3 (2%)	0	100	100
1	C	188/213 (88%)	185 (98%)	3 (2%)	0	100	100
1	D	196/213 (92%)	191 (97%)	5 (3%)	0	100	100
All	All	733/852 (86%)	720 (98%)	13 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

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	196/213 (92%)	0.12	18 (9%) 14 15	10, 22, 70, 85	6 (3%)
1	B	190/213 (89%)	0.05	18 (9%) 14 14	10, 22, 68, 85	4 (2%)
1	C	191/213 (89%)	0.33	30 (15%) 5 5	12, 24, 82, 89	3 (1%)
1	D	199/213 (93%)	0.09	19 (9%) 14 14	10, 21, 66, 79	1 (0%)
All	All	776/852 (91%)	0.15	85 (10%) 10 11	10, 22, 74, 89	14 (1%)

All (85) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	202	GLY	5.8
1	C	198	LEU	5.5
1	D	197	ASN	4.8
1	A	195	LEU	4.3
1	D	190	ALA	4.0
1	A	196	ARG	4.0
1	C	199	VAL	3.9
1	B	180	ALA	3.8
1	C	201	LEU	3.7
1	B	182	SER	3.7
1	B	189	ALA	3.7
1	C	197	ASN	3.6
1	C	13	LEU	3.6
1	D	198	LEU	3.6
1	C	200	ASN	3.4
1	C	1	MET	3.4
1	B	194	MET	3.3
1	C	155	PHE	3.3
1	C	28	VAL	3.3
1	B	19	VAL	3.2
1	D	194	MET	3.2

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Mol	Chain	Res	Type	RSRZ
1	D	25	VAL	3.2
1	C	190	ALA	3.2
1	B	21	GLU	3.1
1	B	191	LEU	3.1
1	D	202	GLY	3.1
1	C	20	LEU	3.1
1	C	16	LEU	3.0
1	A	193	PRO	3.0
1	B	17	SER	2.9
1	A	187	ALA	2.9
1	A	181	VAL	2.9
1	C	194	MET	2.8
1	A	25	VAL	2.8
1	B	28	VAL	2.8
1	D	203	ARG	2.7
1	C	22	SER	2.7
1	C	19	VAL	2.7
1	A	14	ALA	2.7
1	B	183	HIS	2.7
1	C	9	ASN	2.7
1	A	191	LEU	2.6
1	C	153	ASN	2.6
1	A	10	PRO	2.6
1	D	16	LEU	2.6
1	D	189	ALA	2.5
1	B	20	LEU	2.5
1	C	15	GLU	2.5
1	A	194	MET	2.5
1	B	193	PRO	2.4
1	C	14	ALA	2.4
1	D	23	SER	2.4
1	C	174	THR	2.4
1	C	187	ALA	2.4
1	D	191	LEU	2.4
1	B	26	SER	2.4
1	D	196	ARG	2.4
1	C	189	ALA	2.4
1	B	181	VAL	2.4
1	A	180	ALA	2.3
1	C	188	LEU	2.3
1	D	187	ALA	2.3
1	D	154	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	188	LEU	2.3
1	C	26	SER	2.3
1	D	199	VAL	2.3
1	A	189	ALA	2.3
1	C	10	PRO	2.3
1	C	11	LYS	2.3
1	C	192	LEU	2.3
1	B	18	ARG	2.2
1	A	26	SER	2.2
1	D	178	LYS	2.2
1	A	22	SER	2.2
1	C	12	LYS	2.2
1	B	153	ASN	2.1
1	D	193	PRO	2.1
1	A	183	HIS	2.1
1	B	185	GLY	2.1
1	B	190	ALA	2.1
1	A	96	GLY	2.1
1	C	184	ARG	2.0
1	A	27	GLY	2.0
1	A	19	VAL	2.0
1	D	95	HIS	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.