Full wwPDB X-ray Structure Validation Report (i)

Jun 12, 2024 – 09:40 AM EDT

PDB ID	:	2X5S
Title	:	Crystal structure of T. maritima GDP-mannose pyrophosphorylase in apo state.
Authors	:	Pelissier, M.C.; Lesley, S.; Kuhn, P.; Bourne, Y.
Deposited on	:	2010-02-10
Resolution	:	2.35 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 (i) 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 (1)) were used in the production of this report:

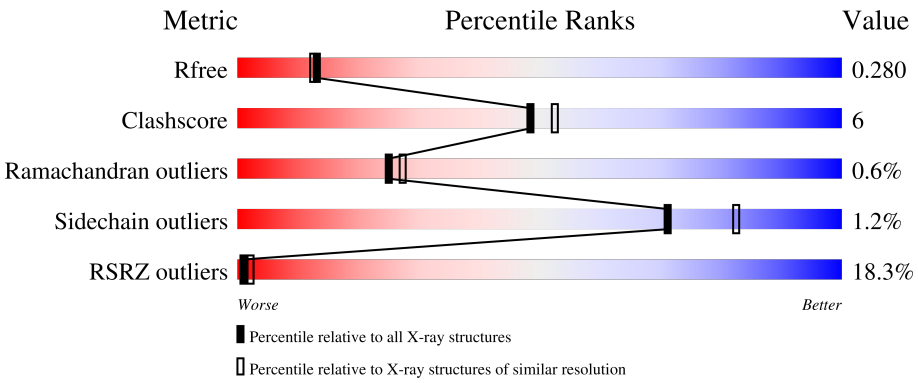
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.20.1
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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	1164 (2.36-2.36)
Clashscore	141614	1232 (2.36-2.36)
Ramachandran outliers	138981	1211 (2.36-2.36)
Sidechain outliers	138945	1212 (2.36-2.36)
RSRZ outliers	127900	1150 (2.36-2.36)

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 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 <=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	336	15% 83% 15%
1	B	336	21% 84% 15%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 5414 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 MANNOSE-1-PHOSPHATE GUANYLYLTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	333	2674	1726	436	503	9	0	0	0
1	B	333	2693	1740	439	505	9	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	VAL	MET	engineered mutation	UNP Q9X0C3
A	261	LEU	VAL	engineered mutation	UNP Q9X0C3
B	1	VAL	MET	engineered mutation	UNP Q9X0C3
B	261	LEU	VAL	engineered mutation	UNP Q9X0C3

- Molecule 2 is water.

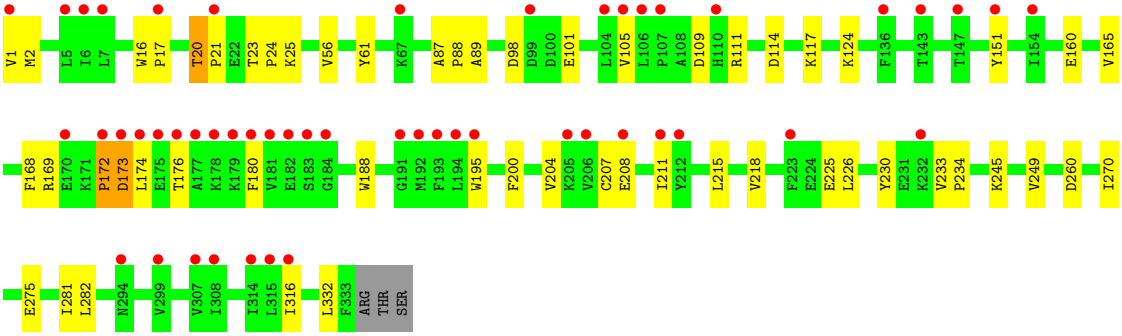
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	A	31	31	31	0	0
2	B	16	16	16	0	0

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.

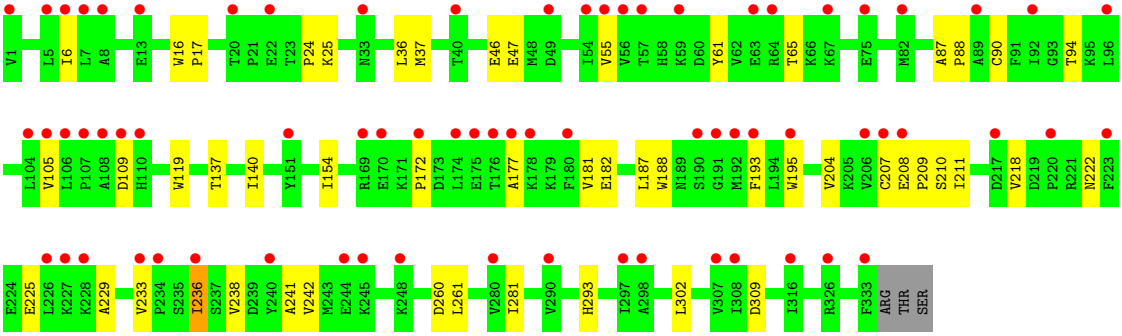
• Molecule 1: MANNOSE-1-PHOSPHATE GUANYLYLTRANSFERASE

Chain A:



• Molecule 1: MANNOSE-1-PHOSPHATE GUANYLYLTRANSFERASE

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	64.01Å 93.00Å 69.69Å 90.00° 110.25° 90.00°	Depositor
Resolution (Å)	65.37 – 2.35 29.49 – 2.35	Depositor EDS
% Data completeness (in resolution range)	99.1 (65.37-2.35) 99.2 (29.49-2.35)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.35 (at 2.36Å)	Xtriage
Refinement program	REFMAC 5.5.0088	Depositor
R, R_{free}	0.224 , 0.273 0.247 , 0.280	Depositor DCC
R_{free} test set	1602 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	54.9	Xtriage
Anisotropy	0.690	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 56.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	5414	wwPDB-VP
Average B, all atoms (Å^2)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.00% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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	0.49	0/2735	0.61	1/3701 (0.0%)
1	B	0.47	0/2754	0.59	1/3722 (0.0%)
All	All	0.48	0/5489	0.60	2/7423 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	172	PRO	N-CA-CB	5.51	109.91	103.30
1	A	172	PRO	N-CA-CB	5.43	109.82	103.30

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	2674	0	2669	33	0
1	B	2693	0	2715	33	0
2	A	31	0	0	0	0
2	B	16	0	0	0	0
All	All	5414	0	5384	64	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 6.

All (64) 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:A:208:GLU:OE2	1:A:245:LYS:NZ	1.86	1.06
1:A:20:THR:HG22	1:A:21:PRO:HD3	1.65	0.79
1:B:87:ALA:HB3	1:B:88:PRO:HD3	1.73	0.71
1:A:20:THR:HG22	1:A:21:PRO:CD	2.23	0.69
1:B:218:VAL:HG13	1:B:225:GLU:HG3	1.79	0.63
1:A:218:VAL:HG13	1:A:225:GLU:HG3	1.83	0.60
1:A:1:VAL:HG12	1:A:1:VAL:O	2.04	0.58
1:B:204:VAL:HG22	1:B:242:VAL:HG21	1.86	0.58
1:A:98:ASP:HB2	1:A:101:GLU:HG3	1.85	0.58
1:B:218:VAL:HG13	1:B:225:GLU:CG	2.33	0.57
1:A:207:CYS:O	1:A:208:GLU:HG2	2.05	0.56
1:A:207:CYS:O	1:A:208:GLU:CG	2.54	0.56
1:A:176:THR:HG22	1:A:180:PHE:CZ	2.41	0.55
1:B:154:ILE:HD11	1:B:187:LEU:CD1	2.38	0.54
1:B:229:ALA:O	1:B:233:VAL:HG23	2.08	0.54
1:A:111:ARG:HD3	1:A:270:ILE:HD13	1.88	0.54
1:A:281:ILE:HD12	1:A:281:ILE:N	2.22	0.54
1:B:177:ALA:O	1:B:181:VAL:HG23	2.07	0.54
1:A:87:ALA:HB3	1:A:88:PRO:HD3	1.89	0.54
1:B:37:MET:HE3	1:B:65:THR:HG23	1.90	0.52
1:A:211:ILE:HG23	1:A:215:LEU:HD12	1.91	0.52
1:B:211:ILE:HD13	1:B:233:VAL:HG13	1.92	0.52
1:A:200:PHE:O	1:A:204:VAL:HG23	2.11	0.51
1:B:90:CYS:O	1:B:94:THR:OG1	2.27	0.50
1:B:207:CYS:O	1:B:208:GLU:OE2	2.30	0.50
1:A:124:LYS:NZ	1:A:160:GLU:O	2.36	0.49
1:A:24:PRO:HG3	1:A:61:TYR:CZ	2.48	0.49
1:B:209:PRO:O	1:B:210:SER:C	2.49	0.49
1:B:25:LYS:HD2	1:B:109:ASP:HB2	1.95	0.49
1:A:151:TYR:N	1:A:169:ARG:O	2.45	0.49
1:A:275:GLU:H	1:A:275:GLU:CD	2.17	0.49
1:B:25:LYS:CD	1:B:109:ASP:HB2	2.43	0.48
1:B:238:VAL:HA	1:B:241:ALA:HB3	1.95	0.48
1:B:281:ILE:HD12	1:B:281:ILE:N	2.29	0.47
1:B:140:ILE:HB	1:B:188:TRP:HB2	1.95	0.47
1:A:316:ILE:HG22	1:B:302:LEU:HD12	1.96	0.46
1:A:316:ILE:HG22	1:B:302:LEU:CD1	2.45	0.46
1:B:260:ASP:OD1	1:B:260:ASP:C	2.54	0.45
1:B:47:GLU:HG3	1:B:119:TRP:CD2	2.51	0.45
1:A:233:VAL:HG13	1:A:234:PRO:HD2	1.97	0.45
1:B:154:ILE:HD11	1:B:187:LEU:HD11	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:165:VAL:HG21	1:A:249:VAL:HG12	1.99	0.44
1:A:114:ASP:OD2	1:A:117:LYS:HG3	2.17	0.44
1:B:236:ILE:HG23	1:B:236:ILE:O	2.17	0.44
1:A:105:VAL:HG21	1:A:195:TRP:CZ2	2.52	0.44
1:B:36:LEU:HD22	1:B:261:LEU:CD1	2.46	0.44
1:A:173:ASP:OD1	1:A:174:LEU:N	2.51	0.43
1:A:25:LYS:HE2	1:A:109:ASP:HB2	2.00	0.43
1:B:16:TRP:CD1	1:B:17:PRO:HA	2.54	0.43
1:A:281:ILE:O	1:A:282:LEU:HD23	2.19	0.43
1:B:16:TRP:CG	1:B:17:PRO:HA	2.53	0.43
1:B:24:PRO:HG3	1:B:61:TYR:CE1	2.53	0.42
1:A:226:LEU:HD11	1:A:230:TYR:CE1	2.54	0.42
1:A:173:ASP:OD1	1:A:174:LEU:O	2.38	0.42
1:A:151:TYR:HH	1:A:188:TRP:HE1	1.67	0.41
1:A:56:VAL:HG11	1:A:89:ALA:HB1	2.03	0.41
1:A:23:THR:HA	1:A:24:PRO:HD3	1.87	0.41
1:B:137:THR:HG22	1:B:193:PHE:CD1	2.55	0.41
1:B:260:ASP:OD1	1:B:261:LEU:N	2.54	0.41
1:A:16:TRP:CG	1:A:17:PRO:HA	2.55	0.41
1:B:47:GLU:HG3	1:B:119:TRP:CG	2.56	0.41
1:B:293:HIS:HB2	1:B:309:ASP:O	2.21	0.41
1:B:105:VAL:HG21	1:B:195:TRP:CZ2	2.56	0.40
1:B:6:ILE:HB	1:B:55:VAL:HG22	2.04	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	331/336 (98%)	319 (96%)	10 (3%)	2 (1%)	25 27
1	B	331/336 (98%)	320 (97%)	9 (3%)	2 (1%)	25 27

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	662/672 (98%)	639 (96%)	19 (3%)	4 (1%)	25 27

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	172	PRO
1	B	236	ILE
1	A	2	MET
1	B	222	ASN

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	292/302 (97%)	287 (98%)	5 (2%)	60 72
1	B	297/302 (98%)	295 (99%)	2 (1%)	84 91
All	All	589/604 (98%)	582 (99%)	7 (1%)	71 82

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	THR
1	A	168	PHE
1	A	173	ASP
1	A	260	ASP
1	A	332	LEU
1	B	46	GLU
1	B	182	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 monosaccharides 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 (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	333/336 (99%)	0.93	51 (15%)	2	3	40, 67, 123, 151	0
1	B	333/336 (99%)	1.14	71 (21%)	0	1	40, 72, 137, 182	0
All	All	666/672 (99%)	1.03	122 (18%)	1	2	40, 69, 128, 182	0

All (122) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	172	PRO	9.9
1	B	178	LYS	7.5
1	B	172	PRO	7.1
1	B	7	LEU	6.5
1	A	174	LEU	6.5
1	B	6	ILE	6.4
1	B	175	GLU	6.1
1	A	143	THR	5.8
1	B	107	PRO	5.7
1	A	177	ALA	5.7
1	B	333	PHE	5.6
1	B	220	PRO	5.6
1	B	106	LEU	5.3
1	A	182	GLU	5.3
1	A	294	ASN	5.3
1	A	105	VAL	5.1
1	A	1	VAL	5.0
1	A	106	LEU	5.0
1	A	178	LYS	4.9
1	A	175	GLU	4.8
1	B	207	CYS	4.8
1	B	105	VAL	4.7
1	A	211	ILE	4.6
1	B	174	LEU	4.6

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Mol	Chain	Res	Type	RSRZ
1	B	5	LEU	4.5
1	B	206	VAL	4.5
1	A	193	PHE	4.4
1	A	191	GLY	4.4
1	A	147	THR	4.3
1	A	173	ASP	4.1
1	B	56	VAL	3.9
1	B	108	ALA	3.9
1	A	184	GLY	3.9
1	B	307	VAL	3.9
1	B	223	PHE	3.9
1	B	193	PHE	3.8
1	B	1	VAL	3.8
1	B	226	LEU	3.8
1	B	244	GLU	3.7
1	A	316	ILE	3.7
1	B	177	ALA	3.7
1	B	82	MET	3.6
1	A	314	ILE	3.4
1	A	179	LYS	3.3
1	B	63	GLU	3.3
1	A	212	TYR	3.3
1	B	170	GLU	3.3
1	A	183	SER	3.3
1	A	307	VAL	3.3
1	A	5	LEU	3.2
1	B	191	GLY	3.2
1	B	190	SER	3.2
1	A	17	PRO	3.2
1	A	192	MET	3.2
1	B	234	PRO	3.1
1	B	180	PHE	3.1
1	A	194	LEU	3.1
1	A	232	LYS	3.1
1	B	240	TYR	3.0
1	B	22	GLU	3.0
1	B	326	ARG	3.0
1	B	96	LEU	2.9
1	A	176	THR	2.9
1	A	7	LEU	2.9
1	B	290	VAL	2.9
1	B	192	MET	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	169	ARG	2.9
1	B	92	ILE	2.9
1	B	236	ILE	2.9
1	B	297	ILE	2.9
1	B	67	LYS	2.8
1	B	55	VAL	2.8
1	A	170	GLU	2.8
1	B	110	HIS	2.8
1	B	40	THR	2.8
1	B	49	ASP	2.7
1	B	176	THR	2.7
1	A	21	PRO	2.7
1	A	180	PHE	2.6
1	A	205	LYS	2.6
1	B	89	ALA	2.6
1	B	208	GLU	2.6
1	B	75	GLU	2.6
1	B	280	VAL	2.6
1	B	316	ILE	2.5
1	B	248	LYS	2.5
1	A	308	ILE	2.5
1	B	217	ASP	2.5
1	B	33	ASN	2.5
1	B	54	ILE	2.5
1	A	151	TYR	2.4
1	A	136	PHE	2.4
1	B	308	ILE	2.4
1	A	181	VAL	2.4
1	B	104	LEU	2.4
1	B	57	THR	2.4
1	B	195	TRP	2.3
1	B	233	VAL	2.3
1	B	245	LYS	2.3
1	B	20	THR	2.3
1	A	195	TRP	2.3
1	A	110	HIS	2.3
1	A	104	LEU	2.2
1	A	299	VAL	2.2
1	B	109	ASP	2.2
1	B	8	ALA	2.2
1	A	208	GLU	2.2
1	A	154	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	227	LYS	2.1
1	B	228	LYS	2.1
1	A	107	PRO	2.1
1	A	99	ASP	2.1
1	B	64	ARG	2.1
1	A	223	PHE	2.1
1	B	151	TYR	2.1
1	B	298	ALA	2.1
1	A	6	ILE	2.0
1	A	315	LEU	2.0
1	B	59	LYS	2.0
1	B	13	GLU	2.0
1	A	206	VAL	2.0
1	A	67	LYS	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 monosaccharides 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.