



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:27 AM GMT

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
<http://wwpdb.org/validation/2016/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
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

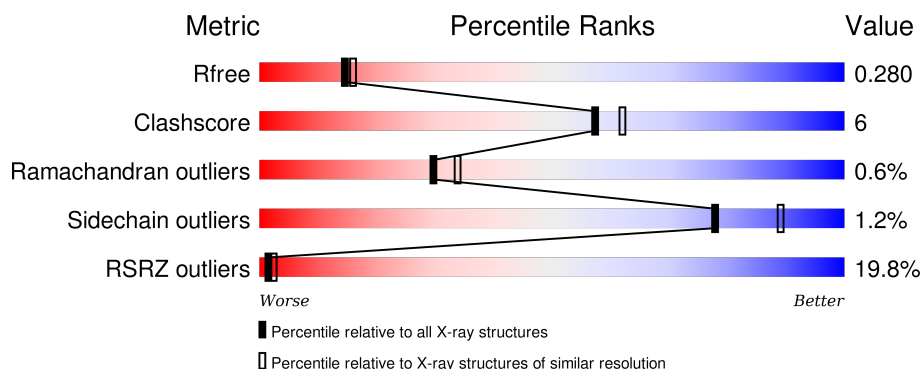
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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}	91344	1352 (2.38-2.34)
Clashscore	102246	1456 (2.38-2.34)
Ramachandran outliers	100387	1435 (2.38-2.34)
Sidechain outliers	100360	1436 (2.38-2.34)
RSRZ outliers	91569	1358 (2.38-2.34)

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. 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	336	<div> <div>16%</div> <div>83%</div> <div>15%</div> <div>..</div> </div>
1	B	336	<div> <div>23%</div> <div>84%</div> <div>15%</div> <div>.</div> </div>

2 Entry composition

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
1	A	333	Total	C	N	O	S	0	0	0
			2674	1726	436	503	9			
1	B	333	Total	C	N	O	S	0	0	0
			2693	1740	439	505	9			

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

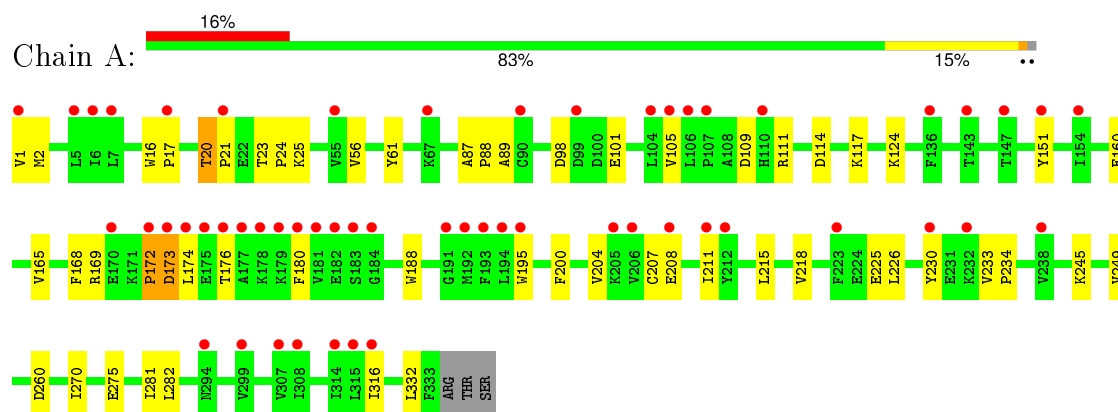
- Molecule 2 is water.

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

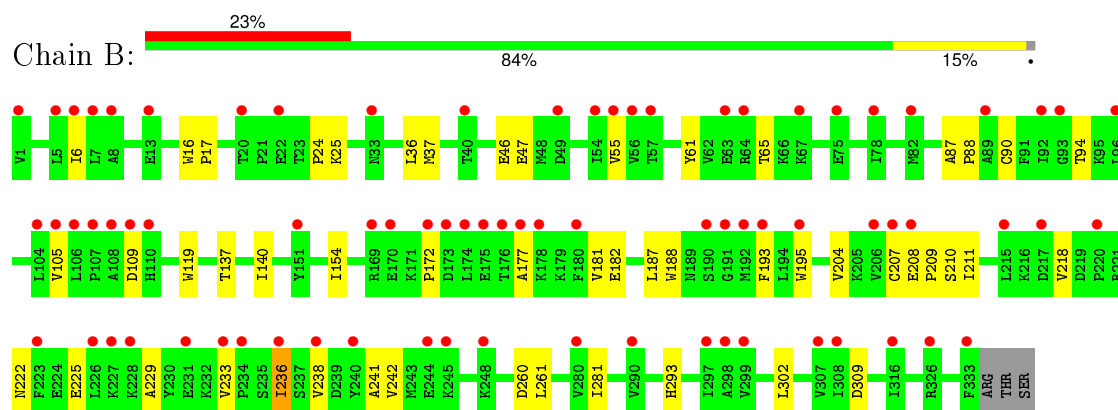
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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: MANNOSE-1-PHOSPHATE GUANYLYLTRANSFERASE



• Molecule 1: MANNOSE-1-PHOSPHATE GUANYLYLTRANSFERASE



4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ 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 (5.32%)	DCC
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
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 31731 reflections	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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(°)	Ideal(°)
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:N	1:A:281:ILE:HD12	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:CD	1:A:275:GLU:H	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:C	1:B:260:ASP:OD1	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:B:36:LEU:HD22	1:B:261:LEU:CD1	2.46	0.44
1:A:105:VAL:HG21	1:A:195:TRP:CZ2	2.52	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:260:ASP:OD1	1:B:261:LEU:N	2.54	0.41
1:B:137:THR:HG22	1:B:193:PHE:CD1	2.55	0.41
1:B:47:GLU:HG3	1:B:119:TRP:CG	2.56	0.41
1:A:16:TRP:CG	1:A:17:PRO:HA	2.55	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%)	30	34
1	B	331/336 (98%)	320 (97%)	9 (3%)	2 (1%)	30	34

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	662/672 (98%)	639 (96%)	19 (3%)	4 (1%)	30	34

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 ⓘ

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%)	68	82
1	B	297/302 (98%)	295 (99%)	2 (1%)	88	95
All	All	589/604 (98%)	582 (99%)	7 (1%)	78	89

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

Some 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 carbohydrates 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	333/336 (99%)	1.01	55 (16%)	2 4	40, 67, 123, 151	0
1	B	333/336 (99%)	1.22	77 (23%)	1 1	40, 72, 137, 182	0
All	All	666/672 (99%)	1.11	132 (19%)	1 2	40, 69, 128, 182	0

All (132) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	172	PRO	10.6
1	B	178	LYS	7.8
1	B	172	PRO	7.6
1	B	7	LEU	6.8
1	A	174	LEU	6.7
1	B	6	ILE	6.7
1	A	143	THR	6.4
1	B	175	GLU	6.2
1	B	107	PRO	5.9
1	B	333	PHE	5.8
1	B	220	PRO	5.7
1	A	177	ALA	5.7
1	A	182	GLU	5.6
1	A	1	VAL	5.6
1	B	106	LEU	5.6
1	A	106	LEU	5.3
1	A	105	VAL	5.2
1	A	294	ASN	5.2
1	A	178	LYS	5.1
1	B	105	VAL	4.9
1	B	207	CYS	4.9
1	A	175	GLU	4.8
1	A	211	ILE	4.8
1	B	206	VAL	4.6

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Mol	Chain	Res	Type	RSRZ
1	B	5	LEU	4.6
1	A	191	GLY	4.5
1	A	193	PHE	4.5
1	B	174	LEU	4.5
1	A	147	THR	4.4
1	A	184	GLY	4.3
1	B	223	PHE	4.3
1	A	173	ASP	4.2
1	B	108	ALA	4.1
1	B	307	VAL	4.1
1	B	1	VAL	4.0
1	B	56	VAL	4.0
1	B	193	PHE	4.0
1	A	316	ILE	4.0
1	B	82	MET	3.8
1	B	226	LEU	3.8
1	B	177	ALA	3.7
1	B	244	GLU	3.7
1	A	314	ILE	3.6
1	B	191	GLY	3.5
1	A	307	VAL	3.5
1	A	212	TYR	3.4
1	B	190	SER	3.4
1	A	17	PRO	3.4
1	A	5	LEU	3.4
1	A	192	MET	3.3
1	B	234	PRO	3.3
1	B	240	TYR	3.3
1	B	180	PHE	3.3
1	A	183	SER	3.2
1	B	169	ARG	3.2
1	A	232	LYS	3.2
1	B	170	GLU	3.2
1	A	179	LYS	3.2
1	B	67	LYS	3.2
1	A	194	LEU	3.1
1	B	96	LEU	3.1
1	B	326	ARG	3.1
1	B	63	GLU	3.1
1	B	55	VAL	3.0
1	B	92	ILE	3.0
1	B	192	MET	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	176	THR	3.0
1	B	22	GLU	3.0
1	B	290	VAL	3.0
1	B	236	ILE	3.0
1	B	297	ILE	3.0
1	A	7	LEU	3.0
1	A	170	GLU	2.9
1	B	40	THR	2.9
1	B	110	HIS	2.9
1	B	89	ALA	2.9
1	A	181	VAL	2.8
1	A	205	LYS	2.8
1	B	176	THR	2.8
1	B	280	VAL	2.7
1	B	208	GLU	2.7
1	A	180	PHE	2.7
1	B	49	ASP	2.7
1	B	316	ILE	2.7
1	A	151	TYR	2.7
1	A	21	PRO	2.7
1	B	57	THR	2.6
1	B	217	ASP	2.6
1	A	136	PHE	2.5
1	B	75	GLU	2.5
1	B	248	LYS	2.5
1	B	104	LEU	2.5
1	B	308	ILE	2.5
1	B	33	ASN	2.5
1	B	8	ALA	2.5
1	B	195	TRP	2.5
1	A	299	VAL	2.5
1	B	233	VAL	2.5
1	A	308	ILE	2.5
1	B	54	ILE	2.5
1	B	20	THR	2.4
1	A	104	LEU	2.4
1	A	110	HIS	2.4
1	B	245	LYS	2.4
1	A	154	ILE	2.4
1	A	107	PRO	2.4
1	A	223	PHE	2.3
1	A	90	CYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	109	ASP	2.3
1	B	151	TYR	2.3
1	B	64	ARG	2.3
1	A	195	TRP	2.3
1	B	298	ALA	2.3
1	B	227	LYS	2.2
1	B	228	LYS	2.2
1	A	206	VAL	2.2
1	A	208	GLU	2.2
1	B	13	GLU	2.2
1	A	6	ILE	2.2
1	A	238	VAL	2.2
1	A	55	VAL	2.1
1	A	99	ASP	2.1
1	B	78	ILE	2.1
1	B	238	VAL	2.1
1	B	299	VAL	2.1
1	B	215	LEU	2.1
1	A	67	LYS	2.1
1	B	173	ASP	2.1
1	B	231	GLU	2.1
1	A	315	LEU	2.0
1	A	230	TYR	2.0
1	B	93	GLY	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 carbohydrates 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.