



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:00 AM UTC

PDB ID : 6EXD / pdb_00006exd
Title : Crystal structure of DotM cytoplasmic domain (residues 153-380) SeMet derivative
Authors : Meir, A.; Waksman, G.
Deposited on : 2017-11-07
Resolution : 2.14 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
Mogul	:	2022.3.0, CSD as543be (2022)
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

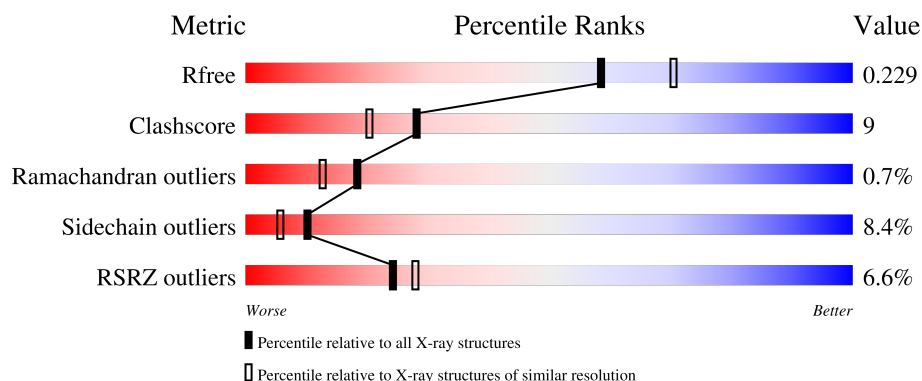
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.14 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	3689 (2.16-2.12)
Clashscore	190562	3812 (2.16-2.12)
Ramachandran outliers	187476	3773 (2.16-2.12)
Sidechain outliers	187428	3772 (2.16-2.12)
RSRZ outliers	180081	3691 (2.16-2.12)

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	235	5% 71% 16% • • 9%
1	B	235	7% 70% 18% 5% • 6%

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 3647 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 IcmP (DotM).

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	214	Total	C	N	O	S	Se	0	2	0
			1746	1111	311	311	2	11			
1	B	220	Total	C	N	O	S	Se	0	0	0
			1770	1127	312	318	2	11			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	146	GLY	-	expression tag	UNP Q5ZYC7
A	147	PRO	-	expression tag	UNP Q5ZYC7
A	148	SER	-	expression tag	UNP Q5ZYC7
A	149	GLY	-	expression tag	UNP Q5ZYC7
A	150	GLY	-	expression tag	UNP Q5ZYC7
A	151	GLY	-	expression tag	UNP Q5ZYC7
A	152	ALA	-	expression tag	UNP Q5ZYC7
B	146	GLY	-	expression tag	UNP Q5ZYC7
B	147	PRO	-	expression tag	UNP Q5ZYC7
B	148	SER	-	expression tag	UNP Q5ZYC7
B	149	GLY	-	expression tag	UNP Q5ZYC7
B	150	GLY	-	expression tag	UNP Q5ZYC7
B	151	GLY	-	expression tag	UNP Q5ZYC7
B	152	ALA	-	expression tag	UNP Q5ZYC7

- Molecule 2 is water.

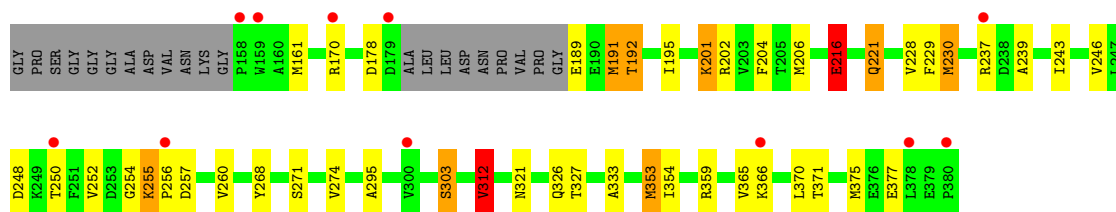
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	73	Total	O	0	0
			73	73		
2	B	58	Total	O	0	0
			58	58		

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.

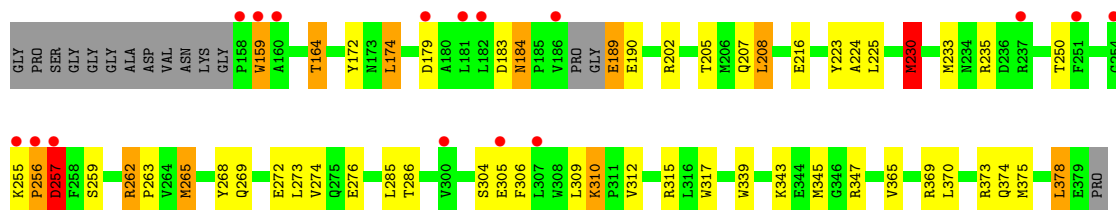
• Molecule 1: IcmP (DotM)

Chain A: 5% 71% 16% • • 9%



• Molecule 1: IcmP (DotM)

Chain B: 7% 70% 18% 5% • 6%



4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α , β , γ	118.00Å 118.00Å 66.40Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.01 – 2.14 50.01 – 2.14	Depositor EDS
% Data completeness (in resolution range)	99.5 (50.01-2.14) 99.7 (50.01-2.14)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.25	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.48 (at 2.14Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.191 , 0.227 0.193 , 0.229	Depositor DCC
R_{free} test set	1469 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	20.9	Xtriage
Anisotropy	0.096	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 37.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.059 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	3647	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.16% 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

5.1 Standard geometry

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	1.21	2/1773 (0.1%)	1.26	7/2374 (0.3%)
1	B	1.22	2/1797 (0.1%)	1.26	9/2410 (0.4%)
All	All	1.22	4/3570 (0.1%)	1.26	16/4784 (0.3%)

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	1
1	B	0	1
All	All	0	2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	248	ASP	N-CA	6.08	1.53	1.46
1	B	257	ASP	CA-C	6.02	1.60	1.52
1	B	256	PRO	CA-C	5.17	1.58	1.52
1	A	327	THR	CA-C	-5.02	1.48	1.52

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	353	MSE	CG-SE-CE	11.60	124.44	98.92
1	B	190	GLU	N-CA-C	7.00	119.76	111.71
1	A	312	VAL	CB-CA-C	-6.61	103.38	112.04
1	B	230	MSE	CB-CA-C	-6.21	100.88	110.81
1	A	191	MSE	CG-SE-CE	5.76	111.59	98.92
1	B	257	ASP	N-CA-C	5.76	119.90	112.41
1	B	304	SER	N-CA-C	5.71	119.98	113.19
1	B	265	MSE	N-CA-C	-5.64	105.21	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	159	TRP	CB-CA-C	-5.57	100.09	109.50
1	B	224	ALA	N-CA-C	5.52	117.29	111.28
1	A	230	MSE	CB-CA-C	-5.50	102.02	110.81
1	A	216	GLU	CB-CG-CD	5.33	121.67	112.60
1	A	228	VAL	CB-CA-C	-5.20	105.12	112.14
1	B	268	TYR	CA-C-N	5.16	127.19	120.28
1	B	268	TYR	C-N-CA	5.16	127.19	120.28
1	A	202	ARG	CG-CD-NE	-5.12	100.74	112.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	254	GLY	Peptide
1	B	256	PRO	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	1746	0	1760	37	1
1	B	1770	0	1782	27	1
2	A	73	0	0	7	0
2	B	58	0	0	2	0
All	All	3647	0	3542	63	1

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 9.

All (63) 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:246:VAL:O	1:A:250:THR:HG22	1.71	0.91
1:A:370:LEU:HD12	1:A:375:MSE:HE2	1.62	0.80
1:A:370:LEU:HB2	1:A:375:MSE:HE2	1.63	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:326:GLN:HB3	2:A:466:HOH:O	1.82	0.77
1:A:216:GLU:HG3	2:A:422:HOH:O	1.87	0.75
1:A:230:MSE:HG2	1:A:274:VAL:HG21	1.68	0.75
1:A:370:LEU:HD12	1:A:375:MSE:CE	2.18	0.73
1:A:370:LEU:HB2	1:A:375:MSE:CE	2.18	0.72
1:A:353:MSE:HE2	2:A:456:HOH:O	1.90	0.71
1:A:216:GLU:CG	2:A:422:HOH:O	2.44	0.61
1:A:250:THR:OG1	1:A:256:PRO:HA	2.00	0.61
1:A:370:LEU:CD1	1:A:375:MSE:HE2	2.29	0.61
1:B:164:THR:HG21	2:B:451:HOH:O	2.00	0.61
1:A:250:THR:CG2	1:A:256:PRO:HA	2.32	0.60
1:A:250:THR:HG21	1:A:257:ASP:H	1.68	0.58
1:A:191:MSE:C	1:A:375:MSE:HE3	2.29	0.57
1:A:237:ARG:NH2	2:A:401:HOH:O	2.27	0.57
1:B:286:THR:HG22	1:B:339:TRP:HB2	1.85	0.57
1:A:250:THR:HB	2:A:442:HOH:O	2.04	0.56
1:B:273:LEU:O	1:B:276:GLU:HG3	2.06	0.56
1:A:370:LEU:CB	1:A:375:MSE:HE2	2.36	0.53
1:B:225:LEU:CD1	1:B:309:LEU:HD22	2.39	0.53
1:B:250:THR:HB	1:B:257:ASP:CG	2.35	0.52
1:B:370:LEU:HB3	1:B:374:GLN:HB2	1.92	0.52
1:A:268:TYR:O	1:A:271:SER:OG	2.26	0.52
1:A:354:ILE:C	1:A:354:ILE:HD12	2.34	0.52
1:B:189:GLU:HA	1:B:189:GLU:OE1	2.09	0.51
1:B:265:MSE:O	1:B:269:GLN:HB2	2.11	0.51
1:B:207:GLN:O	1:B:315:ARG:NH1	2.44	0.50
1:B:223:TYR:CZ	1:B:265:MSE:HG2	2.46	0.50
1:B:310:LYS:HD3	1:B:317:TRP:CD1	2.47	0.50
1:B:375:MSE:O	1:B:378:LEU:HB2	2.12	0.50
1:B:305:GLU:N	1:B:305:GLU:OE2	2.45	0.50
1:B:255:LYS:O	1:B:257:ASP:OD1	2.31	0.48
1:A:206:MSE:HE3	2:A:457:HOH:O	2.13	0.48
1:A:255:LYS:HA	1:A:255:LYS:HD2	1.67	0.48
1:B:233:MSE:HE2	1:B:273:LEU:HB3	1.96	0.48
1:B:250:THR:HG21	1:B:257:ASP:HB3	1.95	0.47
1:A:257:ASP:O	1:A:260:VAL:HG12	2.16	0.46
1:B:259:SER:O	1:B:262:ARG:HG2	2.15	0.46
1:A:250:THR:OG1	1:A:255:LYS:O	2.36	0.44
1:B:273:LEU:HA	1:B:276:GLU:HG2	2.00	0.44
1:A:370:LEU:HB2	1:A:375:MSE:HE3	1.99	0.44
1:A:250:THR:HG23	1:A:256:PRO:HA	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:189:GLU:O	1:A:192:THR:HB	2.18	0.43
1:A:195:ILE:HD11	1:A:365:VAL:HG21	2.01	0.43
1:A:303:SER:HG	1:A:321:ASN:CG	2.26	0.43
1:A:201:LYS:HG2	1:A:354:ILE:HD11	2.02	0.42
1:A:221:GLN:HG2	1:A:312:VAL:HG11	2.02	0.42
1:B:235:ARG:HG2	2:B:429:HOH:O	2.19	0.42
1:B:205:THR:O	1:B:208:LEU:HB2	2.19	0.42
1:A:239:ALA:O	1:A:243:ILE:HG12	2.20	0.41
1:B:183:ASP:O	1:B:184:ASN:HB2	2.20	0.41
1:A:204:PHE:CE1	1:A:333:ALA:HB3	2.56	0.41
1:A:229:PHE:HB3	1:A:295:ALA:HB2	2.03	0.41
1:A:371:THR:CG2	1:B:369:ARG:HD2	2.50	0.41
1:B:230:MSE:CG	1:B:274:VAL:HG21	2.50	0.41
1:A:230:MSE:HG2	1:A:274:VAL:CG2	2.45	0.40
1:B:183:ASP:O	1:B:184:ASN:CB	2.70	0.40
1:A:326:GLN:CD	1:A:326:GLN:H	2.29	0.40
1:B:172:TYR:O	1:B:174:LEU:HD13	2.21	0.40
1:B:345:MSE:CE	1:B:347:ARG:CZ	2.99	0.40
1:B:285:LEU:HD11	1:B:315:ARG:HD2	2.03	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:189:GLU:OE2	1:B:202:ARG:CZ[4_674]	2.15	0.05

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	212/235 (90%)	202 (95%)	8 (4%)	2 (1%)	14 8

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	216/235 (92%)	205 (95%)	10 (5%)	1 (0%)	24	19
All	All	428/470 (91%)	407 (95%)	18 (4%)	3 (1%)	18	13

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	184	ASN
1	A	303	SER
1	A	377	GLU

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	184/184 (100%)	171 (93%)	13 (7%)	13	8
1	B	187/184 (102%)	168 (90%)	19 (10%)	7	3
All	All	371/368 (101%)	339 (91%)	32 (9%)	10	5

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	161	MSE
1	A	170[A]	ARG
1	A	170[B]	ARG
1	A	178	ASP
1	A	192	THR
1	A	201	LYS
1	A	216	GLU
1	A	221	GLN
1	A	252	VAL
1	A	255	LYS
1	A	312	VAL
1	A	359	ARG
1	A	366	LYS

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Mol	Chain	Res	Type
1	B	159	TRP
1	B	164	THR
1	B	174	LEU
1	B	179	ASP
1	B	189	GLU
1	B	208	LEU
1	B	216	GLU
1	B	230	MSE
1	B	257	ASP
1	B	262	ARG
1	B	263	PRO
1	B	272	GLU
1	B	306	PHE
1	B	310	LYS
1	B	312	VAL
1	B	343	LYS
1	B	365	VAL
1	B	373	ARG
1	B	378	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	234	ASN
1	B	234	ASN
1	B	321	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

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

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	203/235 (86%)	0.08	11 (5%) 31 36	8, 26, 55, 89	2 (0%)
1	B	209/235 (88%)	0.29	16 (7%) 19 22	10, 28, 67, 100	0
All	All	412/470 (87%)	0.19	27 (6%) 24 28	8, 27, 64, 100	2 (0%)

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	159	TRP	5.3
1	A	158	PRO	4.4
1	B	256	PRO	4.2
1	B	158	PRO	3.9
1	B	182	LEU	3.9
1	B	186	VAL	3.7
1	B	160	ALA	3.5
1	A	159	TRP	3.4
1	B	181	LEU	3.2
1	B	254	GLY	3.2
1	A	380	PRO	3.1
1	B	300	VAL	2.9
1	A	256	PRO	2.9
1	A	179	ASP	2.7
1	B	179	ASP	2.5
1	A	378	LEU	2.4
1	B	251	PHE	2.4
1	A	300	VAL	2.4
1	B	305	GLU	2.4
1	B	255	LYS	2.4
1	B	307	LEU	2.3
1	B	257	ASP	2.2
1	A	237	ARG	2.1
1	A	250	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	366	LYS	2.1
1	B	237	ARG	2.0
1	A	170[A]	ARG	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.