



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 12:08 PM UTC

PDB ID : 5X9C / pdb_00005x9c
Title : Crystal structure of the cytosolic domain of human MiD51
Authors : Sun, F.; Pang, X.; Ma, J.
Deposited on : 2017-03-06
Resolution : 1.85 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

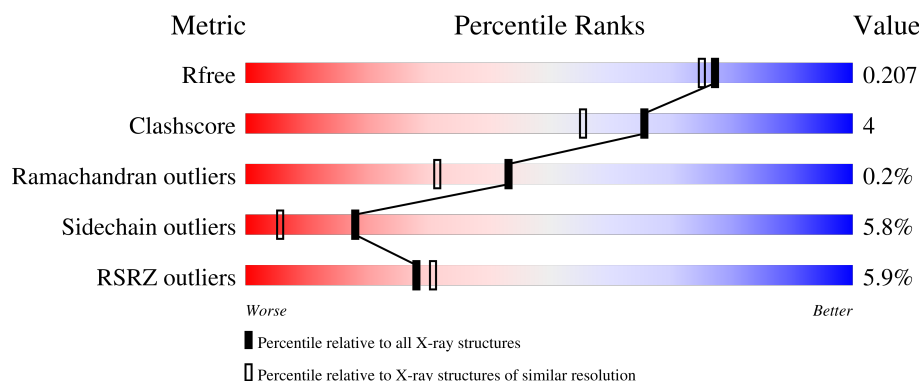
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.85 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	3428 (1.86-1.86)
Clashscore	190562	3579 (1.86-1.86)
Ramachandran outliers	187476	3553 (1.86-1.86)
Sidechain outliers	187428	3553 (1.86-1.86)
RSRZ outliers	180081	3429 (1.86-1.86)

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	336	5% 84% 12% ..
1	B	336	7% 79% 16% ..

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5385 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 Mitochondrial dynamics protein MID51.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	330	Total	C	N	O	S	0	0	0
			2592	1663	435	483	11			
1	B	330	Total	C	N	O	S	0	0	0
			2592	1662	436	483	11			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	128	GLY	-	expression tag	UNP Q9NQG6
A	129	PRO	-	expression tag	UNP Q9NQG6
A	130	LEU	-	expression tag	UNP Q9NQG6
A	131	GLY	-	expression tag	UNP Q9NQG6
A	132	SER	-	expression tag	UNP Q9NQG6
B	128	GLY	-	expression tag	UNP Q9NQG6
B	129	PRO	-	expression tag	UNP Q9NQG6
B	130	LEU	-	expression tag	UNP Q9NQG6
B	131	GLY	-	expression tag	UNP Q9NQG6
B	132	SER	-	expression tag	UNP Q9NQG6

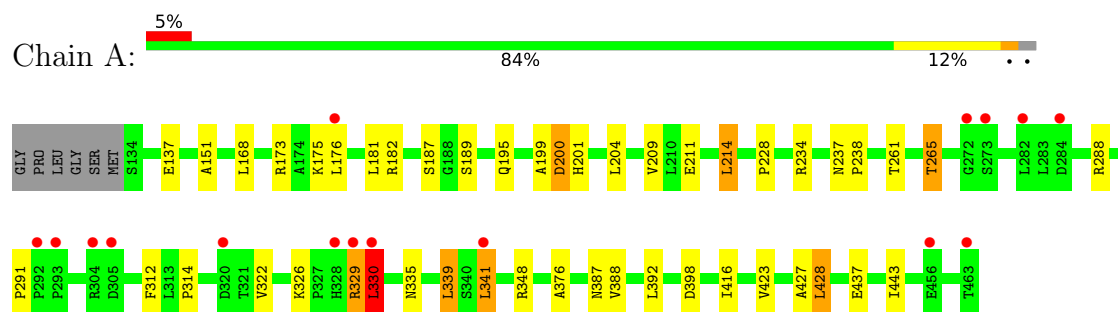
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	112	Total	O	0	0
			112	112		
2	B	89	Total	O	0	0
			89	89		

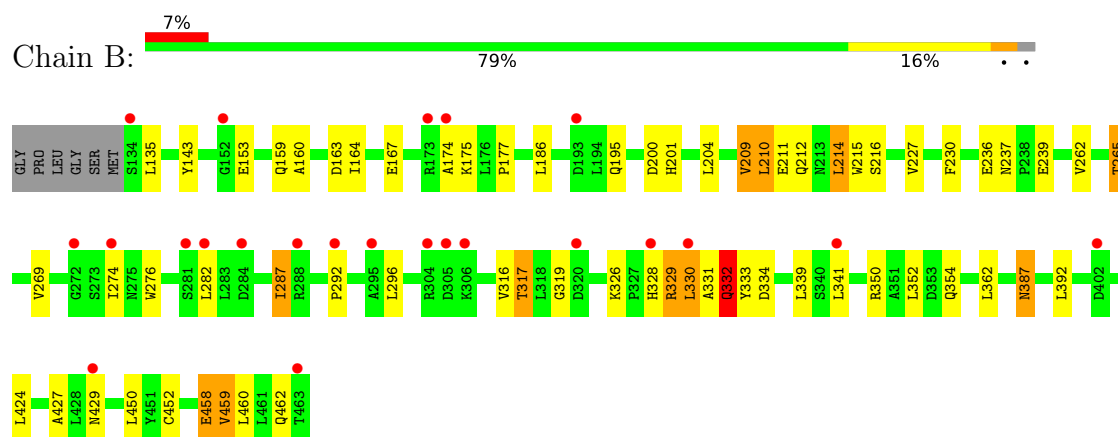
3 Residue-property plots [i](#)

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: Mitochondrial dynamics protein MID51



- Molecule 1: Mitochondrial dynamics protein MID51



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	61.30Å 64.67Å 65.91Å 89.81° 108.08° 117.19°	Depositor
Resolution (Å)	48.54 – 1.85 48.54 – 1.85	Depositor EDS
% Data completeness (in resolution range)	95.3 (48.54-1.85) 97.4 (48.54-1.85)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.00 (at 1.71Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.203 , 0.232 0.207 , 0.207	Depositor DCC
R_{free} test set	4259 reflections (4.63%)	wwPDB-VP
Wilson B-factor (Å ²)	25.6	Xtriage
Anisotropy	0.502	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 28.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5385	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.10% 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	1.49	16/2651 (0.6%)	1.28	10/3617 (0.3%)
1	B	1.48	13/2651 (0.5%)	1.23	9/3618 (0.2%)
All	All	1.49	29/5302 (0.5%)	1.25	19/7235 (0.3%)

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	237	ASN	C-O	-16.18	1.16	1.23
1	B	237	ASN	C-O	8.55	1.27	1.23
1	B	292	PRO	CA-C	8.51	1.56	1.51
1	A	291	PRO	CA-C	7.93	1.56	1.51
1	B	160	ALA	N-CA	-7.43	1.37	1.46
1	A	234	ARG	C-O	-6.92	1.15	1.24
1	A	228	PRO	C-O	-6.91	1.16	1.23
1	B	200	ASP	N-CA	-6.58	1.39	1.46
1	A	314	PRO	C-O	6.27	1.30	1.23
1	A	388	VAL	C-O	6.22	1.31	1.24
1	B	186	LEU	N-CA	5.81	1.53	1.46
1	A	173	ARG	C-O	-5.72	1.17	1.24
1	B	239	GLU	N-CA	5.72	1.53	1.46
1	B	230	PHE	C-O	5.63	1.30	1.23
1	B	153	GLU	C-O	-5.55	1.17	1.24
1	A	437	GLU	N-CA	5.55	1.53	1.46
1	A	189	SER	C-O	-5.51	1.17	1.24
1	B	215	TRP	C-O	-5.48	1.17	1.23
1	A	238	PRO	N-CD	5.45	1.55	1.47
1	A	339	LEU	C-O	-5.38	1.17	1.23
1	B	332	GLN	CD-NE2	5.36	1.44	1.33
1	A	189	SER	CA-C	-5.33	1.45	1.52
1	B	174	ALA	C-O	-5.33	1.18	1.24
1	A	137	GLU	CA-C	5.25	1.59	1.52
1	B	339	LEU	C-O	-5.22	1.17	1.24
1	A	376	ALA	N-CA	5.17	1.52	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	237	ASN	C-N	5.10	1.40	1.34
1	A	398	ASP	C-O	-5.03	1.18	1.24
1	B	339	LEU	N-CA	-5.01	1.39	1.46

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	209	VAL	CG1-CB-CG2	7.24	126.73	110.80
1	A	200	ASP	N-CA-C	6.86	121.63	112.30
1	B	174	ALA	N-CA-C	6.68	118.35	111.14
1	A	291	PRO	N-CA-C	6.43	116.65	110.47
1	B	135	LEU	N-CA-C	-6.32	104.39	111.28
1	A	175	LYS	N-CA-C	6.13	121.04	113.50
1	A	341	LEU	CA-CB-CG	5.92	137.00	116.30
1	A	416	ILE	N-CA-C	5.88	116.06	110.42
1	B	159	GLN	N-CA-C	5.84	117.73	111.36
1	A	182	ARG	CG-CD-NE	-5.82	99.20	112.00
1	B	287	ILE	O-C-N	-5.79	117.01	123.26
1	B	282	LEU	N-CA-C	5.56	117.34	111.28
1	A	187	SER	CA-CB-OG	-5.42	100.27	111.10
1	A	443	ILE	N-CA-C	5.24	115.96	110.62
1	B	387	ASN	N-CA-C	5.22	117.88	111.82
1	A	339	LEU	CB-CG-CD2	5.18	126.23	110.70
1	B	460	LEU	N-CA-C	5.17	118.69	112.38
1	A	288	ARG	N-CA-C	5.09	114.16	108.25
1	B	334	ASP	N-CA-C	5.04	117.42	111.33

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	2592	0	2610	15	0
1	B	2592	0	2603	25	1
2	A	112	0	0	2	2

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	89	0	0	3	1
All	All	5385	0	5213	39	2

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 (39) 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:335:ASN:OD1	2:A:601:HOH:O	2.11	0.68
1:A:387:ASN:HD22	1:A:427:ALA:H	1.49	0.61
1:B:317:THR:HG22	2:B:644:HOH:O	2.00	0.60
1:B:387:ASN:ND2	1:B:427:ALA:H	2.00	0.60
1:B:387:ASN:HD22	1:B:427:ALA:H	1.48	0.60
1:A:265:THR:HG21	2:A:708:HOH:O	2.01	0.59
1:B:329:ARG:HB3	1:B:330:LEU:HD13	1.86	0.57
1:B:195:GLN:HE22	1:B:201:HIS:H	1.56	0.54
1:B:212:GLN:HE22	1:B:319:GLY:H	1.55	0.54
1:A:168:LEU:HD22	1:A:312:PHE:CE2	2.43	0.53
1:A:387:ASN:ND2	1:A:427:ALA:H	2.07	0.53
1:B:459:VAL:HG22	1:B:462:GLN:NE2	2.24	0.52
1:B:274:ILE:HG21	1:B:276:TRP:CZ2	2.46	0.50
1:B:210:LEU:HD22	1:B:316:VAL:HB	1.93	0.50
1:B:204:LEU:C	1:B:204:LEU:HD23	2.37	0.49
1:A:329:ARG:O	1:A:330:LEU:CB	2.60	0.49
1:A:261:THR:O	1:A:265:THR:HG23	2.13	0.48
1:B:458:GLU:HG2	2:B:641:HOH:O	2.15	0.46
1:B:212:GLN:NE2	1:B:319:GLY:H	2.13	0.46
1:B:216:SER:OG	1:B:236:GLU:OE2	2.23	0.45
1:B:163:ASP:O	1:B:167:GLU:HG2	2.17	0.45
1:B:227:VAL:HG13	1:B:333:TYR:HE1	1.82	0.45
1:A:195:GLN:NE2	1:A:200:ASP:H	2.16	0.44
1:B:211:GLU:HB2	1:B:214:LEU:HB2	1.98	0.44
1:B:331:ALA:O	1:B:332:GLN:C	2.60	0.44
1:A:329:ARG:O	1:A:330:LEU:HB3	2.17	0.44
1:A:211:GLU:HB2	1:A:214:LEU:HB2	2.00	0.43
1:A:195:GLN:HE21	1:A:199:ALA:HA	1.84	0.43
1:A:151:ALA:CB	1:B:177:PRO:HB2	2.49	0.43
1:B:143:TYR:CD2	1:B:362:LEU:HD11	2.54	0.42
1:A:195:GLN:HE22	1:A:201:HIS:H	1.68	0.42
1:B:265:THR:HG21	2:B:688:HOH:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:348:ARG:NH2	1:A:428:LEU:HD13	2.34	0.41
1:A:204:LEU:HD23	1:A:204:LEU:C	2.46	0.41
1:B:274:ILE:CG2	1:B:276:TRP:CE2	3.04	0.41
1:B:326:LYS:O	1:B:328:HIS:CE1	2.73	0.41
1:B:350:ARG:O	1:B:354:GLN:HB2	2.20	0.41
1:B:164:ILE:HD11	1:B:287:ILE:HD13	2.03	0.41
1:B:262:VAL:O	1:B:265:THR:HG23	2.21	0.41

All (2) 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)
2:A:703:HOH:O	2:B:686:HOH:O[1_546]	1.58	0.62
1:B:452:CYS:SG	2:A:697:HOH:O[1_564]	2.08	0.12

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	328/336 (98%)	324 (99%)	3 (1%)	1 (0%)	36	25
1	B	328/336 (98%)	323 (98%)	5 (2%)	0	100	100
All	All	656/672 (98%)	647 (99%)	8 (1%)	1 (0%)	43	31

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	330	LEU

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	283/288 (98%)	269 (95%)	14 (5%)	22	8
1	B	282/288 (98%)	263 (93%)	19 (7%)	15	4
All	All	565/576 (98%)	532 (94%)	33 (6%)	18	6

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	176	LEU
1	A	181	LEU
1	A	209	VAL
1	A	214	LEU
1	A	265	THR
1	A	322	VAL
1	A	326	LYS
1	A	329	ARG
1	A	330	LEU
1	A	339	LEU
1	A	341	LEU
1	A	392	LEU
1	A	423	VAL
1	A	428	LEU
1	B	175	LYS
1	B	209	VAL
1	B	210	LEU
1	B	214	LEU
1	B	265	THR
1	B	269	VAL
1	B	296	LEU
1	B	317	THR
1	B	329	ARG
1	B	330	LEU
1	B	332	GLN
1	B	341	LEU
1	B	352	LEU

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Mol	Chain	Res	Type
1	B	392	LEU
1	B	424	LEU
1	B	429	ASN
1	B	450	LEU
1	B	458	GLU
1	B	459	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	154	GLN
1	A	195	GLN
1	A	203	GLN
1	A	387	ASN
1	A	429	ASN
1	B	145	ASN
1	B	154	GLN
1	B	195	GLN
1	B	212	GLN
1	B	275	ASN
1	B	387	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 [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	330/336 (98%)	0.19	16 (4%) 35 39	7, 19, 40, 51	0
1	B	330/336 (98%)	0.31	23 (6%) 22 24	10, 21, 43, 53	0
All	All	660/672 (98%)	0.25	39 (5%) 28 31	7, 20, 42, 53	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	329	ARG	5.8
1	A	284	ASP	5.0
1	B	304	ARG	4.8
1	A	305	ASP	4.2
1	A	292	PRO	3.7
1	B	282	LEU	3.5
1	A	304	ARG	3.5
1	A	293	PRO	3.3
1	B	429	ASN	3.3
1	B	274	ILE	3.0
1	B	328	HIS	3.0
1	B	281	SER	3.0
1	A	330	LEU	2.9
1	A	328	HIS	2.8
1	B	173	ARG	2.7
1	B	134	SER	2.7
1	A	176	LEU	2.6
1	A	282	LEU	2.6
1	A	320	ASP	2.6
1	A	341	LEU	2.6
1	B	305	ASP	2.6
1	B	272	GLY	2.6
1	A	272	GLY	2.5
1	B	292	PRO	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	341	LEU	2.4
1	B	284	ASP	2.4
1	B	295	ALA	2.4
1	B	402	ASP	2.4
1	A	463	THR	2.3
1	B	463	THR	2.3
1	B	288	ARG	2.2
1	B	152	GLY	2.2
1	A	456	GLU	2.2
1	B	320	ASP	2.2
1	B	306	LYS	2.2
1	A	273	SER	2.1
1	B	174	ALA	2.1
1	B	193	ASP	2.1
1	B	330	LEU	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.