



# Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 05:24 pm BST

PDB ID : 6N73  
Title : Crystal Structure of ATPase delta1-79 Spa47 R271A  
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Deposited on : 2018-11-27  
Resolution : 2.40 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](mailto: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.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
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) : 2.11

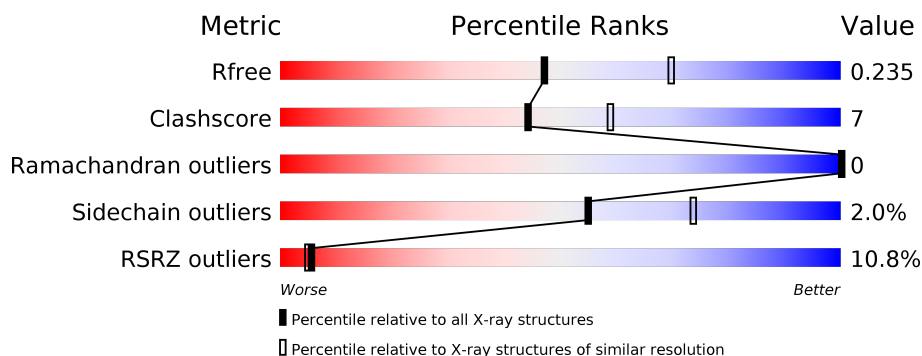
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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  $\geq 3$ , 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	352	<div> <div>12%</div> <div> <div></div> <div>78%</div> <div>16%</div> <div>• 5%</div> </div> </div>
1	B	352	<div> <div>9%</div> <div> <div></div> <div>82%</div> <div>12%</div> <div>• 6%</div> </div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5267 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 ATP synthase SpaL/MxiB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	335	Total	C	N	O	S	0	1	0
			2628	1674	445	500	9			
1	B	331	Total	C	N	O	S	0	0	0
			2581	1638	441	493	9			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	79	ASN	-	expression tag	UNP P0A1C1
A	271	ALA	ARG	engineered mutation	UNP P0A1C1
B	79	ASN	-	expression tag	UNP P0A1C1
B	271	ALA	ARG	engineered mutation	UNP P0A1C1

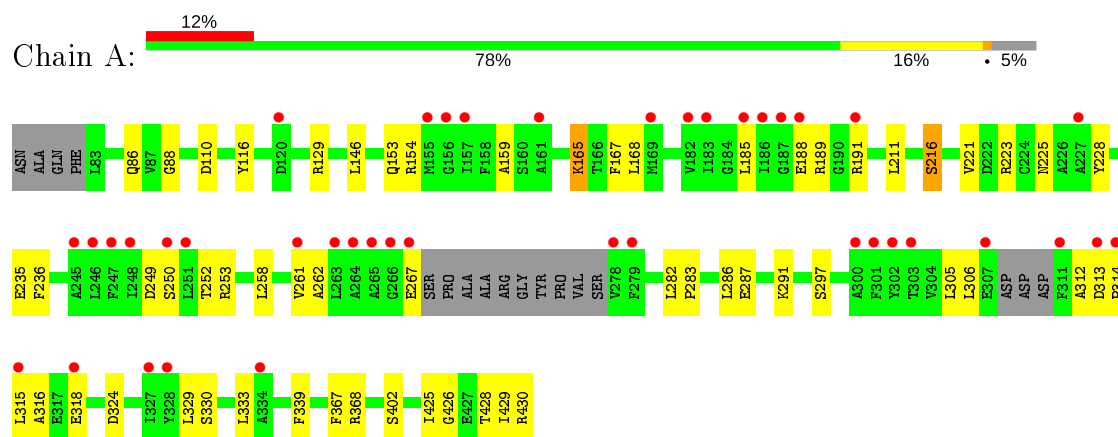
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	30	Total	O	0	0
			30	30		
2	B	28	Total	O	0	0
			28	28		

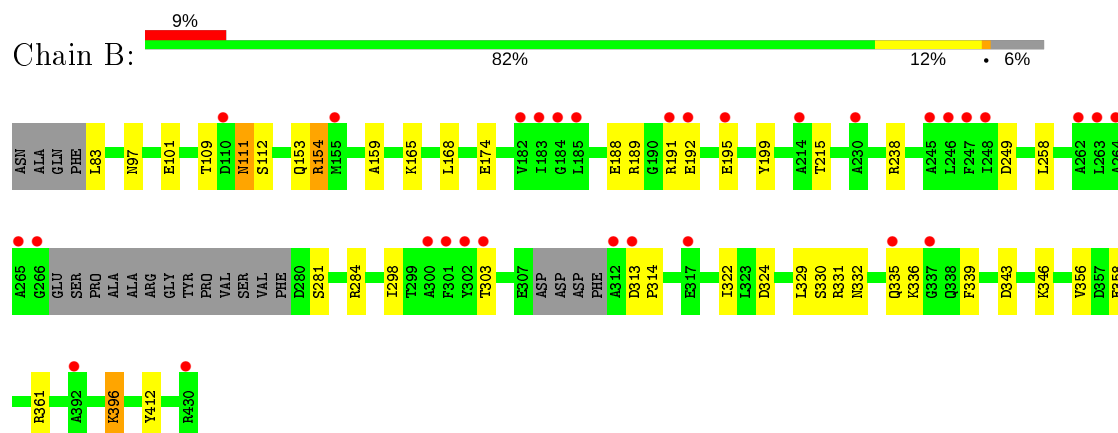
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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: ATP synthase SpaL/MxiB



- Molecule 1: ATP synthase SpaL/MxiB



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	44.20 Å 154.12 Å 54.91 Å 90.00° 110.03° 90.00°	Depositor
Resolution (Å)	32.30 – 2.40 32.29 – 2.40	Depositor EDS
% Data completeness (in resolution range)	96.3 (32.30-2.40) 92.5 (32.29-2.40)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.83 (at 2.39 Å)	Xtriage
Refinement program	PHENIX 1.13 _2998	Depositor
R, $R_{free}$	0.185 , 0.235 0.185 , 0.235	Depositor DCC
$R_{free}$ test set	1301 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	55.3	Xtriage
Anisotropy	0.272	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 44.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	5267	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.02% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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	0.29	0/2674	0.49	0/3609
1	B	0.28	0/2621	0.46	0/3537
All	All	0.28	0/5295	0.47	0/7146

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

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	2628	0	2646	43	0
1	B	2581	0	2604	27	0
2	A	30	0	0	1	0
2	B	28	0	0	0	0
All	All	5267	0	5250	69	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 7.

All (69) 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:313:ASP:OD1	1:B:314:PRO:HD2	1.44	1.18

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:192:GLU:HA	1:B:195:GLU:HG2	1.54	0.90
1:A:189:ARG:HH21	1:A:191:ARG:HH12	1.31	0.77
1:A:129:ARG:NH2	1:A:287:GLU:O	2.19	0.75
1:A:314:PRO:O	1:A:318:GLU:HG2	1.87	0.74
1:B:313:ASP:CG	1:B:314:PRO:HD2	2.07	0.74
1:B:153:GLN:HG3	1:B:324:ASP:HB2	1.69	0.73
1:B:343:ASP:OD2	1:B:346:LYS:HD2	1.94	0.68
1:B:258:LEU:HD21	1:B:281:SER:HB3	1.77	0.67
1:A:235:GLU:OE2	2:A:501:HOH:O	2.13	0.65
1:B:165:LYS:NZ	1:B:249:ASP:OD1	2.27	0.64
1:B:165:LYS:HE2	1:B:303:THR:HG21	1.80	0.63
1:A:146:LEU:O	1:A:368:ARG:NH2	2.31	0.63
1:A:291:LYS:HG2	1:A:297:SER:HB3	1.82	0.61
1:A:225:ASN:HA	1:A:228:TYR:HD1	1.66	0.61
1:A:425:ILE:O	1:A:428:THR:HG22	2.01	0.60
1:B:356:VAL:O	1:B:361:ARG:NH2	2.35	0.59
1:A:221:VAL:O	1:A:225:ASN:ND2	2.35	0.59
1:A:262:ALA:HB1	1:A:267:GLU:HB2	1.83	0.58
1:A:189:ARG:HH21	1:A:191:ARG:NH1	2.02	0.56
1:A:153:GLN:HG3	1:A:324:ASP:HB2	1.87	0.56
1:B:191:ARG:HB3	1:B:192:GLU:OE1	2.05	0.56
1:B:109:THR:HG22	1:B:111:ASN:H	1.72	0.54
1:B:396:LYS:HD2	1:B:396:LYS:H	1.71	0.54
1:A:305:LEU:HD13	1:A:306:LEU:N	2.23	0.53
1:A:154:ARG:HD2	1:A:286:LEU:O	2.09	0.53
1:A:165:LYS:H	1:A:165:LYS:HD3	1.74	0.53
1:B:188:GLU:HA	1:B:188:GLU:OE1	2.08	0.52
1:B:396:LYS:HD2	1:B:396:LYS:N	2.24	0.52
1:A:312:ALA:HB1	1:A:316:ALA:HB3	1.92	0.52
1:A:165:LYS:HD3	1:A:165:LYS:N	2.24	0.52
1:B:111:ASN:HD22	1:B:112:SER:N	2.09	0.51
1:B:174:GLU:HG2	1:B:199:TYR:OH	2.10	0.51
1:A:262:ALA:HB1	1:A:267:GLU:CB	2.41	0.50
1:B:331:ARG:O	1:B:335:GLN:HG2	2.11	0.50
1:A:282:LEU:O	1:A:286:LEU:HG	2.11	0.50
1:A:367:PHE:CE1	1:A:428:THR:HG21	2.48	0.49
1:A:88:GLY:HA2	1:A:236:PHE:CE2	2.48	0.49
1:A:252:THR:HA	1:A:315:LEU:HD21	1.96	0.48
1:B:238:ARG:HD3	1:B:298:ILE:HG13	1.95	0.47
1:A:225:ASN:HA	1:A:228:TYR:CD1	2.48	0.47
1:A:188:GLU:HG3	1:A:216:SER:HB2	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:282:LEU:HB3	1:A:283:PRO:HD3	1.96	0.47
1:A:429:ILE:HD12	1:A:430:ARG:HD3	1.97	0.47
1:A:249:ASP:HA	1:A:250:SER:HA	1.66	0.47
1:B:188:GLU:O	1:B:215:THR:HA	2.16	0.46
1:A:86:GLN:HG2	1:A:116:TYR:CE2	2.52	0.45
1:A:146:LEU:HD11	1:A:367:PHE:CD2	2.52	0.45
1:A:189:ARG:NE	1:A:189:ARG:HA	2.31	0.45
1:A:167:PHE:HB3	1:A:339:PHE:CZ	2.52	0.45
1:B:159:ALA:HB2	1:B:329:LEU:HB2	2.00	0.44
1:A:330:SER:HB3	1:A:333:LEU:HB2	1.99	0.44
1:A:258:LEU:O	1:A:261:VAL:HG12	2.18	0.43
1:A:283:PRO:O	1:A:287:GLU:HG2	2.18	0.43
1:B:97:ASN:OD1	1:B:101:GLU:HG3	2.19	0.43
1:A:110:ASP:OD2	1:B:358:GLU:HG2	2.19	0.42
1:A:159:ALA:HB2	1:A:329:LEU:HB2	2.00	0.42
1:A:313:ASP:CG	1:A:315:LEU:H	2.23	0.42
1:B:154:ARG:NH2	1:B:322:ILE:O	2.51	0.42
1:A:189:ARG:NH2	1:A:191:ARG:HH12	2.08	0.41
1:A:216:SER:HA	1:A:223:ARG:NH2	2.36	0.41
1:B:165:LYS:NZ	1:B:249:ASP:CG	2.74	0.41
1:A:165:LYS:H	1:A:165:LYS:CD	2.34	0.41
1:B:168:LEU:HD22	1:B:329:LEU:HD21	2.04	0.40
1:A:185:LEU:HG	1:A:211:LEU:HD11	2.03	0.40
1:A:168:LEU:HD22	1:A:329:LEU:HD21	2.03	0.40
1:A:426:GLY:O	1:A:430:ARG:HG2	2.21	0.40
1:B:332:ASN:O	1:B:336:LYS:HG3	2.22	0.40
1:B:339:PHE:CE2	1:B:412:TYR:HB3	2.57	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	330/352 (94%)	325 (98%)	5 (2%)	0	100	100
1	B	325/352 (92%)	319 (98%)	6 (2%)	0	100	100
All	All	655/704 (93%)	644 (98%)	11 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	281/293 (96%)	277 (99%)	4 (1%)	67	82
1	B	276/293 (94%)	269 (98%)	7 (2%)	47	67
All	All	557/586 (95%)	546 (98%)	11 (2%)	55	74

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	165	LYS
1	A	216	SER
1	A	253	ARG
1	A	402	SER
1	B	83	LEU
1	B	111	ASN
1	B	154	ARG
1	B	189	ARG
1	B	284	ARG
1	B	330	SER
1	B	396	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	225	ASN
1	B	111	ASN

### 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	335/352 (95%)	0.61	41 (12%) 4 3	39, 63, 109, 161	0
1	B	331/352 (94%)	0.49	31 (9%) 8 7	39, 64, 107, 144	0
All	All	666/704 (94%)	0.55	72 (10%) 5 5	39, 63, 108, 161	0

All (72) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	311	PHE	6.3
1	A	265	ALA	5.4
1	B	266	GLY	5.0
1	B	430	ARG	4.8
1	A	278	VAL	4.5
1	A	266	GLY	4.0
1	B	312	ALA	3.9
1	B	262	ALA	3.8
1	A	186	ILE	3.8
1	B	192	GLU	3.7
1	A	246	LEU	3.7
1	A	328[A]	TYR	3.7
1	B	246	LEU	3.6
1	A	314	PRO	3.6
1	B	182	VAL	3.6
1	B	313	ASP	3.6
1	A	247	PHE	3.5
1	A	187	GLY	3.5
1	A	307	GLU	3.4
1	A	301	PHE	3.3
1	B	191	ARG	3.2
1	B	248	ILE	3.2
1	A	248	ILE	3.2
1	B	263	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	300	ALA	3.2
1	A	191	ARG	3.2
1	A	267	GLU	3.1
1	A	279	PHE	3.1
1	B	337	GLY	3.1
1	A	250	SER	3.0
1	B	335	GLN	3.0
1	B	183	ILE	3.0
1	B	195	GLU	2.9
1	B	301	PHE	2.9
1	A	183	ILE	2.8
1	B	184	GLY	2.8
1	A	263	LEU	2.7
1	A	182	VAL	2.7
1	B	247	PHE	2.7
1	B	302	TYR	2.6
1	B	155	MET	2.6
1	A	302	TYR	2.6
1	A	313	ASP	2.6
1	A	334	ALA	2.5
1	A	120	ASP	2.5
1	A	251	LEU	2.5
1	B	110	ASP	2.4
1	A	188	GLU	2.4
1	A	185	LEU	2.4
1	A	264	ALA	2.4
1	B	317	GLU	2.4
1	A	156	GLY	2.3
1	A	155	MET	2.3
1	B	185	LEU	2.3
1	B	303	THR	2.3
1	A	300	ALA	2.3
1	B	265	ALA	2.3
1	A	169	MET	2.2
1	A	318	GLU	2.2
1	B	214	ALA	2.2
1	A	227	ALA	2.2
1	A	303	THR	2.2
1	B	230	ALA	2.2
1	A	327	ILE	2.1
1	A	161	ALA	2.1
1	A	315	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	245	ALA	2.1
1	B	264	ALA	2.1
1	A	245	ALA	2.1
1	A	261	VAL	2.1
1	B	392	ALA	2.0
1	A	157	ILE	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.