



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 25, 2024 – 09:53 PM EDT

PDB ID : 7LCY  
Title : Crystal structure of the ligand-free ARM domain from Drosophila SARM1  
Authors : Gu, W.; Nanson, J.D.; Luo, Z.; McGuinness, H.Y.; Manik, M.K.; Jia, X.; Ve, T.; Kobe, B.  
Deposited on : 2021-01-12  
Resolution : 3.35 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](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.

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	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
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)	:	2.37.1

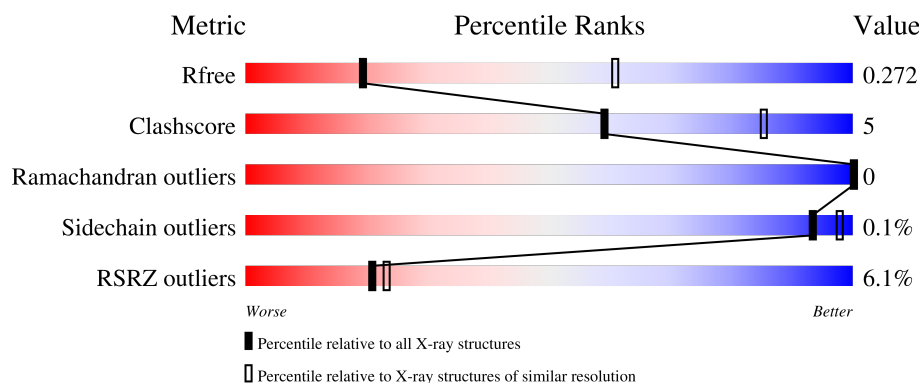
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.35 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	1558 (3.42-3.30)
Clashscore	141614	1627 (3.42-3.30)
Ramachandran outliers	138981	1599 (3.42-3.30)
Sidechain outliers	138945	1598 (3.42-3.30)
RSRZ outliers	127900	1507 (3.42-3.30)

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  $\geq 3$ , 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	367	<div> <div>3%</div> <div>79%</div> <div>11%</div> <div>10%</div> </div>
1	B	367	<div> <div>5%</div> <div>76%</div> <div>8%</div> <div>16%</div> </div>
1	C	367	<div> <div>7%</div> <div>77%</div> <div>10%</div> <div>14%</div> </div>

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 7424 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 Isoform B of NAD(+) hydrolase sarm1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	331	Total	C	N	O	S	0	0	0
			2561	1601	459	483	18			
1	B	310	Total	C	N	O	S	0	0	0
			2400	1500	431	451	18			
1	C	317	Total	C	N	O	S	0	0	0
			2463	1541	441	463	18			

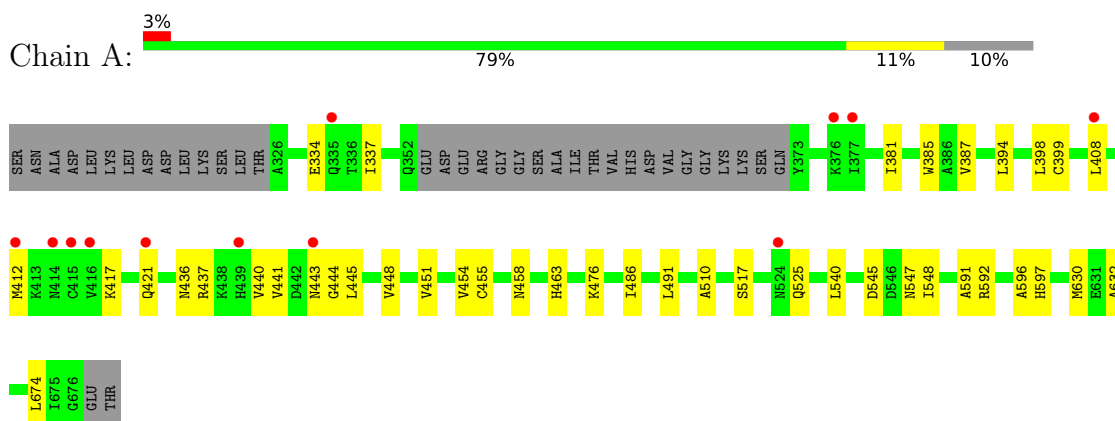
There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	312	SER	-	expression tag	UNP Q6IDD9
A	313	ASN	-	expression tag	UNP Q6IDD9
B	312	SER	-	expression tag	UNP Q6IDD9
B	313	ASN	-	expression tag	UNP Q6IDD9
C	312	SER	-	expression tag	UNP Q6IDD9
C	313	ASN	-	expression tag	UNP Q6IDD9

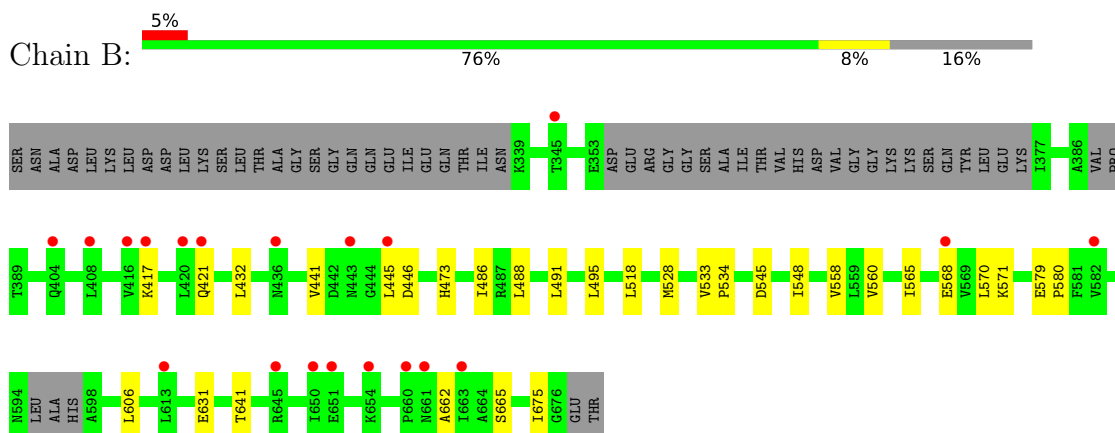
### 3 Residue-property plots [i](#)

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.

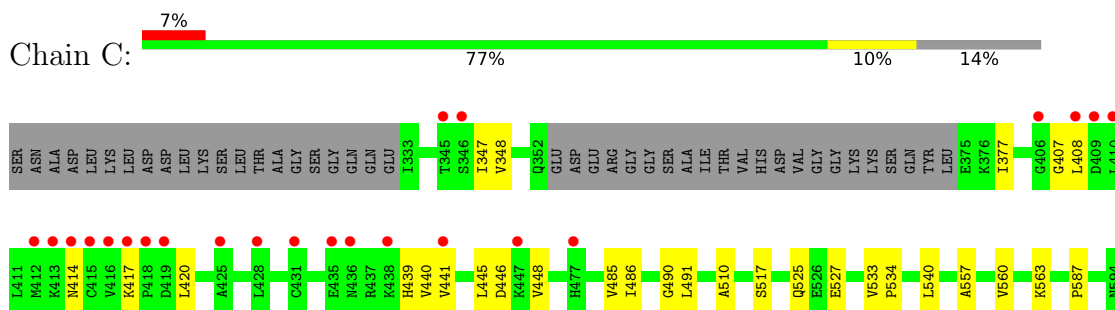
- Molecule 1: Isoform B of NAD(+) hydrolase sarm1

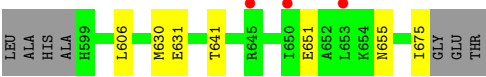


- Molecule 1: Isoform B of NAD(+) hydrolase sarm1



- Molecule 1: Isoform B of NAD(+) hydrolase sarm1





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	63.30Å 101.36Å 98.57Å 90.00° 103.77° 90.00°	Depositor
Resolution (Å)	47.87 – 3.35 47.87 – 3.35	Depositor EDS
% Data completeness (in resolution range)	98.1 (47.87-3.35) 98.1 (47.87-3.35)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.04 (at 3.33Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, $R_{free}$	0.244 , 0.272 0.244 , 0.272	Depositor DCC
$R_{free}$ test set	791 reflections (4.61%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	86.4	Xtriage
Anisotropy	0.340	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 48.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	7424	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	90.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.16% 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 [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	0.23	0/2603	0.38	0/3517
1	B	0.23	0/2437	0.37	0/3288
1	C	0.23	0/2502	0.37	0/3379
All	All	0.23	0/7542	0.37	0/10184

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 [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	2561	0	2551	23	0
1	B	2400	0	2390	25	0
1	C	2463	0	2461	21	0
All	All	7424	0	7402	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 5.

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:570:LEU:HD12	1:B:571:LYS:N	1.89	0.86

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:570:LEU:HD12	1:B:571:LYS:HG3	1.61	0.80
1:C:606:LEU:HD11	1:C:631:GLU:HG2	1.66	0.76
1:B:570:LEU:CD1	1:B:571:LYS:HG3	2.17	0.74
1:B:570:LEU:CD1	1:B:571:LYS:N	2.57	0.67
1:A:441:VAL:HG13	1:A:445:LEU:HD22	1.82	0.61
1:A:592:ARG:HA	1:A:596:ALA:HB2	1.82	0.61
1:C:651:GLU:O	1:C:655:ASN:ND2	2.33	0.61
1:B:570:LEU:HD12	1:B:571:LYS:CG	2.31	0.60
1:A:591:ALA:HB2	1:A:630:MET:HG3	1.83	0.59
1:C:517:SER:O	1:C:525:GLN:NE2	2.36	0.58
1:C:641:THR:HB	1:C:675:ILE:HG23	1.84	0.58
1:B:570:LEU:CD1	1:B:571:LYS:H	2.16	0.58
1:B:432:LEU:HD23	1:B:473:HIS:HB2	1.86	0.57
1:B:560:VAL:HG12	1:B:560:VAL:O	2.06	0.55
1:B:641:THR:HB	1:B:675:ILE:HG23	1.89	0.54
1:B:545:ASP:OD2	1:B:548:ILE:HG13	2.10	0.52
1:A:381:ILE:HG12	1:A:398:LEU:HD23	1.90	0.52
1:A:486:ILE:HG12	1:A:491:LEU:HB2	1.90	0.52
1:B:606:LEU:HD11	1:B:631:GLU:HG2	1.92	0.52
1:A:458:ASN:HD21	1:A:463:HIS:HB3	1.76	0.51
1:A:399:CYS:HB3	1:A:436:ASN:HD21	1.77	0.50
1:A:517:SER:O	1:A:525:GLN:NE2	2.37	0.50
1:C:441:VAL:HG22	1:C:445:LEU:HD13	1.94	0.50
1:C:560:VAL:O	1:C:563:LYS:HG2	2.13	0.49
1:A:437:ARG:NH1	1:A:476:LYS:O	2.46	0.48
1:B:662:ALA:HA	1:B:665:SER:HB3	1.95	0.48
1:A:440:VAL:HG13	1:A:448:VAL:HG21	1.95	0.48
1:A:510:ALA:HB2	1:A:540:LEU:HD23	1.95	0.47
1:B:441:VAL:HG22	1:B:445:LEU:HD13	1.96	0.47
1:C:417:LYS:HD2	1:C:420:LEU:HD12	1.96	0.47
1:A:591:ALA:O	1:A:596:ALA:HB2	2.15	0.46
1:B:486:ILE:HG12	1:B:491:LEU:HB2	1.96	0.46
1:A:443:ASN:OD1	1:A:444:GLY:N	2.48	0.46
1:A:455:CYS:O	1:A:458:ASN:ND2	2.49	0.46
1:C:486:ILE:HG12	1:C:491:LEU:HB2	1.97	0.46
1:B:565:ILE:HG13	1:B:568:GLU:HB2	1.97	0.46
1:C:408:LEU:HD23	1:C:439:HIS:CD2	2.52	0.45
1:B:518:LEU:HD23	1:B:558:VAL:HG11	1.98	0.45
1:C:446:ASP:OD1	1:C:446:ASP:N	2.49	0.45
1:B:441:VAL:HA	1:B:445:LEU:HB2	1.98	0.45
1:B:417:LYS:O	1:B:421:GLN:HG3	2.18	0.44

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:528:MET:HE2	1:B:533:VAL:HG21	1.99	0.44
1:B:495:LEU:HD11	1:B:533:VAL:HG22	2.00	0.43
1:B:560:VAL:O	1:B:560:VAL:CG1	2.66	0.43
1:A:385:TRP:O	1:A:597:HIS:NE2	2.52	0.43
1:C:510:ALA:HB2	1:C:540:LEU:HD23	2.01	0.43
1:C:440:VAL:HG13	1:C:448:VAL:HG21	2.00	0.43
1:A:545:ASP:OD2	1:A:547:ASN:HB3	2.18	0.43
1:C:441:VAL:HG13	1:C:445:LEU:HD22	2.00	0.43
1:C:485:VAL:HG12	1:C:490:GLY:HA3	2.01	0.42
1:C:557:ALA:O	1:C:560:VAL:HG22	2.18	0.42
1:A:334:GLU:HG3	1:A:337:ILE:HD12	2.00	0.42
1:B:579:GLU:HB3	1:B:580:PRO:HD3	2.02	0.42
1:C:348:VAL:HG11	1:C:407:GLY:HA2	2.02	0.42
1:A:451:VAL:HA	1:A:454:VAL:HG22	2.02	0.42
1:B:446:ASP:HA	1:B:488:LEU:HD13	2.03	0.41
1:A:545:ASP:OD2	1:A:548:ILE:HG13	2.20	0.41
1:B:432:LEU:HD12	1:B:432:LEU:HA	1.94	0.41
1:A:408:LEU:O	1:A:412:MET:HG3	2.21	0.41
1:A:417:LYS:O	1:A:421:GLN:HG3	2.21	0.41
1:C:486:ILE:HG21	1:C:527:GLU:HG2	2.02	0.41
1:C:651:GLU:OE1	1:C:651:GLU:N	2.46	0.41
1:C:347:ILE:HD13	1:C:377:ILE:HG21	2.02	0.41
1:C:533:VAL:N	1:C:534:PRO:HD2	2.36	0.41
1:C:587:PRO:O	1:C:630:MET:HG2	2.21	0.40
1:A:632:ALA:HB1	1:A:674:LEU:HB2	2.02	0.40
1:B:533:VAL:N	1:B:534:PRO:HD2	2.36	0.40
1:A:387:VAL:HG21	1:A:394:LEU:HD22	2.02	0.40

There are no symmetry-related clashes.

## 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	327/367 (89%)	313 (96%)	14 (4%)	0	100	100
1	B	302/367 (82%)	284 (94%)	18 (6%)	0	100	100
1	C	311/367 (85%)	299 (96%)	12 (4%)	0	100	100
All	All	940/1101 (85%)	896 (95%)	44 (5%)	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	280/310 (90%)	280 (100%)	0	100	100
1	B	263/310 (85%)	263 (100%)	0	100	100
1	C	272/310 (88%)	271 (100%)	1 (0%)	91	95
All	All	815/930 (88%)	814 (100%)	1 (0%)	93	98

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	414	ASN

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

### 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 [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 ⓘ

### 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	331/367 (90%)	0.36	12 (3%)	42 45	51, 80, 116, 160	0
1	B	310/367 (84%)	0.50	20 (6%)	18 21	51, 89, 133, 171	0
1	C	317/367 (86%)	0.63	26 (8%)	11 13	51, 92, 139, 186	0
All	All	958/1101 (87%)	0.49	58 (6%)	21 23	51, 86, 133, 186	0

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	412	MET	7.8
1	B	661	ASN	6.0
1	C	447	LYS	5.9
1	C	415	CYS	4.7
1	A	376	LYS	4.3
1	A	415	CYS	3.8
1	C	345	THR	3.8
1	C	418	PRO	3.7
1	B	645	ARG	3.7
1	C	406	GLY	3.4
1	C	419	ASP	3.4
1	C	425	ALA	3.3
1	C	417	LYS	3.3
1	B	404	GLN	3.2
1	B	660	PRO	3.2
1	C	409	ASP	3.2
1	C	435	GLU	3.1
1	C	477	HIS	2.9
1	B	443	ASN	2.9
1	A	524	ASN	2.8
1	B	436	ASN	2.8
1	C	436	ASN	2.8
1	B	408	LEU	2.7

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	C	410	LEU	2.7
1	A	421	GLN	2.7
1	C	653	LEU	2.5
1	B	416	VAL	2.5
1	C	346	SER	2.5
1	C	413	LYS	2.4
1	B	345	THR	2.4
1	A	408	LEU	2.4
1	C	645	ARG	2.4
1	B	650	ILE	2.4
1	B	568	GLU	2.4
1	A	335	GLN	2.4
1	B	663	ILE	2.4
1	A	443	ASN	2.4
1	C	416	VAL	2.3
1	B	420	LEU	2.3
1	C	414	ASN	2.3
1	B	445	LEU	2.3
1	A	439	HIS	2.3
1	B	582	VAL	2.3
1	C	408	LEU	2.3
1	B	421	GLN	2.2
1	B	654	LYS	2.2
1	C	428	LEU	2.2
1	A	416	VAL	2.2
1	B	651	GLU	2.2
1	C	431	CYS	2.2
1	B	417	LYS	2.2
1	C	650	ILE	2.2
1	A	414	ASN	2.2
1	A	412	MET	2.1
1	C	438	LYS	2.1
1	A	377	ILE	2.1
1	C	441	VAL	2.0
1	B	613	LEU	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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.