

# Full wwPDB X-ray Structure Validation Report (i)

Oct 20, 2024 – 10:29 PM EDT

PDB ID : 9CQJ

Title : CRYSTAL STRUCTURE OF GAGA-DOG HSP47(36-418) IN COMPLEX

WITH ADNECTIN-53

Authors : Sheriff, S. Deposited on : 2024-07-19

Resolution : 2.08 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 (i) 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 (1)) were used in the production of this report:

MolProbity : 4.02b-467 Xtriage (Phenix) : 1.20.1

EDS : 3.0

Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)

CCP4 : 9.0.003 (Gargrove)

Density-Fitness : 1.0.11

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

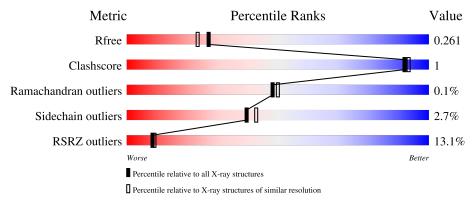
Validation Pipeline (wwPDB-VP) : 2.39

# 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: X- $RAY\ DIFFRACTION$ 

The reported resolution of this entry is 2.08 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 $(\# \mathrm{Entries})$	$\begin{array}{c} {\rm Similar\ resolution} \\ (\#{\rm Entries},{\rm resolution\ range}(\mathring{\rm A})) \end{array}$
$R_{free}$	164625	7574 (2.10-2.06)
Clashscore	180529	8325 (2.10-2.06)
Ramachandran outliers	177936	8271 (2.10-2.06)
Sidechain outliers	177891	8272 (2.10-2.06)
RSRZ outliers	164620	7574 (2.10-2.06)

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 <=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	387	12%	5% • •
1	В	387	91%	6% •
2	D	103	11% 89%	• 7%
2	Е	103	12%	• • 8%



# 2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 14354 atoms, of which 7024 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 Serpin H1.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace			
1	A	380	Total 5753	C 1851	H 2851	N 498	O 540	S 13	2851	0	0
1	В	377	Total 5715	C 1840	H 2837	N 490	O 536	S 12	2837	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	32	GLY	-	expression tag	UNP C7C419
A	33	ALA	-	expression tag	UNP C7C419
A	34	GLY	-	expression tag	UNP C7C419
A	35	ALA	-	expression tag	UNP C7C419
В	32	GLY	-	expression tag	UNP C7C419
В	33	ALA	-	expression tag	UNP C7C419
В	34	GLY	-	expression tag	UNP C7C419
В	35	ALA	-	expression tag	UNP C7C419

• Molecule 2 is a protein called anti-HSP47 Adnectin-53.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
2	D	96	Total	С	Н	N	О	671	0	0
2	D	90	1396	463	671	118	144	071	U	U
2	E	95	Total	С	Н	N	О	665	0	0
2	15	99	1380	456	665	117	142	005	U	U

• Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	48	Total O 49 49	0	1
3	В	25	Total O 25 25	0	0



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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	D	19	Total O 19 19	0	0
3	E	17	Total O 17 17	0	0



# 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: Serpin H1 Chain A: • Molecule 1: Serpin H1 Chain B: 91% • Molecule 2: anti-HSP47 Adnectin-53 Chain D: 89% • Molecule 2: anti-HSP47 Adnectin-53 Chain E:







# 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants	86.81Å 129.06Å 78.22Å	Donositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	78.22 - 2.08	Depositor
Resolution (A)	78.22 - 2.08	EDS
% Data completeness	87.2 (78.22-2.08)	Depositor
(in resolution range)	87.2 (78.22-2.08)	EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) > 1$	1.61 (at 2.07Å)	Xtriage
Refinement program	BUSTER 2.11.8	Depositor
D D.	0.248 , 0.273	Depositor
$R, R_{free}$	0.240 , 0.261	DCC
$R_{free}$ test set	2359 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	48.5	Xtriage
Anisotropy	0.018	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$ , $B_{sol}(Å^2)$	0.36, 38.0	EDS
L-test for twinning <sup>2</sup>	$ < L > = 0.49, < L^2> = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	14354	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.24% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;sup>2</sup>Theoretical values of <|L|>,  $<L^2>$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



<sup>&</sup>lt;sup>1</sup>Intensities estimated from amplitudes.

# 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	Mol Chain		lengths	Bond angles		
IVIOI	Chain	RMSZ	# Z  > 5	RMSZ	# Z  > 5	
1	A	0.41	0/2962	0.60	0/4009	
1	В	0.41	0/2938	0.59	0/3977	
2	D	0.41	0/747	0.61	0/1029	
2	Е	0.42	0/736	0.61	0/1014	
All	All	0.41	0/7383	0.60	0/10029	

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	2902	2851	2852	8	1
1	В	2878	2837	2837	9	0
2	D	725	671	671	1	1
2	Е	715	665	665	3	0
3	A	49	0	0	0	0
3	В	25	0	0	1	0
3	D	19	0	0	0	0
3	Е	17	0	0	0	0
All	All	7330	7024	7025	21	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 1.



All (21) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

A + 1	A + a 2	Interatomic	Clash
Atom-1	Atom-2	${\rm distance}(\mathring{\rm A})$	overlap (Å)
1:A:250:LYS:O	1:A:252:LYS:HE3	1.99	0.62
1:B:250:LYS:O	1:B:252:LYS:HE3	2.00	0.61
1:B:290:LEU:O	1:B:294:MET:HG2	2.02	0.60
2:E:43:GLY:O	2:E:46:PRO:HD3	2.03	0.58
1:B:220:ASP:OD1	1:B:222:ARG:HD3	2.04	0.58
1:A:220:ASP:OD1	1:A:222:ARG:HD3	2.03	0.58
1:B:144:GLU:O	1:B:148:ARG:HG2	2.05	0.57
1:A:58:MET:HE1	1:A:315:HIS:CE1	2.43	0.54
2:D:80:GLU:O	2:D:85:GLY:HA3	2.10	0.52
2:E:80:GLU:O	2:E:85:GLY:HA3	2.11	0.50
1:A:271:MET:SD	1:A:384:ALA:HA	2.53	0.49
1:B:247:ASP:OD1	1:B:273:HIS:NE2	2.40	0.49
1:B:271:MET:SD	1:B:384:ALA:HA	2.54	0.47
1:A:44:ALA:HB2	1:A:114:LEU:HD21	1.96	0.46
1:A:58:MET:CE	1:A:315:HIS:ND1	2.79	0.45
1:B:44:ALA:HB2	1:B:114:LEU:HD21	1.99	0.45
1:B:208:PRO:HD2	1:B:358:GLU:O	2.18	0.44
1:B:112:GLY:HA3	3:B:516:HOH:O	2.19	0.43
1:A:58:MET:CE	1:A:315:HIS:CE1	3.02	0.42
1:A:171:GLN:O	1:A:175:GLU:HG2	2.19	0.41
2:E:6:VAL:O	2:E:8:ARG:HD3	2.20	0.41

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	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	$\begin{array}{c} \text{Clash} \\ \text{overlap } (\text{\AA}) \end{array}$
1:A:133:ARG:HH22	2:D:55:GLU:OE1[2_555]	1.47	0.13

## 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	Perce	entiles
1	A	378/387 (98%)	362 (96%)	15 (4%)	1 (0%)	37	36
1	В	375/387 (97%)	360 (96%)	15 (4%)	0	100	100
2	D	94/103 (91%)	92 (98%)	2 (2%)	0	100	100
2	E	93/103 (90%)	90 (97%)	3 (3%)	0	100	100
All	All	940/980 (96%)	904 (96%)	35 (4%)	1 (0%)	48	50

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	410	LYS

#### 5.3.2 Protein sidechains (i)

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	Perce	ntiles
1	A	300/328 (92%)	291 (97%)	9 (3%)	36	38
1	В	298/328 (91%)	290 (97%)	8 (3%)	40	43
2	D	74/86 (86%)	73 (99%)	1 (1%)	62	68
2	E	73/86 (85%)	71 (97%)	2 (3%)	40	43
All	All	745/828 (90%)	725 (97%)	20 (3%)	40	43

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	68	LEU
1	A	86	LYS
1	A	97	LEU
1	A	133	ARG
1	A	134	LEU
1	A	152	GLN
1	A	252	LYS
1	A	253	LEU
1	A	330	ILE
1	В	68	LEU



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Mol	Chain	Res	Type
1	В	97	LEU
1	В	133	ARG
1	В	134	LEU
1	В	252	LYS
1	В	253	LEU
1	В	330	ILE
1	В	391	LEU
2	D	6	VAL
2	Е	6	VAL
2	Е	8	ARG

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	152	GLN
1	A	368	GLN
1	В	209	HIS

#### 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 oligosaccharides 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 (i)

#### 6.1 Protein, DNA and RNA chains (i)

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,  $95^{th}$  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 $>$	$\# \mathrm{RSRZ}{>}2$	$OWAB(Å^2)$	Q<0.9
1	A	380/387 (98%)	0.79	45 (11%) 10 11	15, 26, 48, 59	0
1	В	377/387 (97%)	0.91	56 (14%) 7 7	16, 28, 52, 65	0
2	D	96/103 (93%)	1.03	11 (11%) 11 12	18, 28, 48, 60	0
2	E	95/103 (92%)	1.03	12 (12%) 9 10	17, 28, 45, 55	0
All	All	948/980 (96%)	0.89	124 (13%) 8 9	15, 27, 50, 65	0

All (124) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	163	PHE	5.4
1	В	126	VAL	5.3
1	A	99	ALA	4.5
1	В	342	GLY	4.4
2	D	42	GLY	4.4
2	D	4	SER	4.4
1	A	96	VAL	4.3
2	Е	45	SER	4.3
1	В	122	THR	4.3
2	D	45	SER	4.2
1	В	163	PHE	4.0
2	Е	99	HIS	4.0
1	В	125	ASN	3.9
1	В	346	LEU	3.9
1	В	145	ASP	3.8
2	Е	5	ASP	3.7
1	В	326	LEU	3.7
1	В	198	ALA	3.6
2	Е	43	GLY	3.6
1	В	119	SER	3.5
2	D	96	THR	3.5



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Mol	Chain	Res	Type	RSRZ
1	В	170	LEU	3.4
2	Е	96	THR	3.3
1	A	372	GLY	3.3
1	В	188	VAL	3.2
1	В	123	ALA	3.2
1	В	118	LEU	3.2
1	A	375	GLU	3.2
1	A	192	VAL	3.1
1	В	287	LYS	3.1
1	A	414	MET	3.0
1	A	195	THR	3.0
2	D	44	ASN	3.0
2	D	46	PRO	2.9
1	В	329	ALA	2.9
1	A	94	LYS	2.9
1	В	337	LEU	2.9
1	В	348	LEU	2.9
1	A	97	LEU	2.9
1	A	329	ALA	2.9
1	В	120	ASN	2.9
1	В	371	TYR	2.9
2	D	5	ASP	2.8
1	В	376	LEU	2.8
1	A	331	ASP	2.7
1	В	121	SER	2.7
2	Е	44	ASN	2.7
1	В	343	LYS	2.7
1	A	102	LEU	2.7
1	В	142	PHE	2.7
1	В	124	ARG	2.7
1	A	370	ILE	2.7
1	В	330	ILE	2.7
2	D	99	HIS	2.7
1	A	188	VAL	2.6
1	В	35	ALA	2.6
1	A	88	THR	2.6
1	В	375	GLU	2.6
1	A	119	SER	2.6
1	A	376	LEU	2.6
1	В	40	ALA	2.6
1	A	170	LEU	2.6
2	D	13	VAL	2.5



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Mol     Chain     Res     Type     RSRZ       2     E     46     PRO     2.5       1     A     161     ILE     2.5       1     B     370     ILE     2.5       1     B     199     LEU     2.5       1     B     34     GLY     2.5       1     A     196     ASP     2.5       1     B     369     ASP     2.5       1     B     369     ASP     2.5       1     B     369     ASP     2.5       1     A     140     VAL     2.5       1     A     333     ASN     2.4       1     B     324     LEU     2.4       1     B     327     THR     2.4 <th></th> <th>nued fron</th> <th></th> <th></th> <th></th>		nued fron			
1     A     161     ILE     2.5       1     B     370     ILE     2.5       1     B     199     LEU     2.5       1     B     34     GLY     2.5       1     A     196     ASP     2.5       1     B     369     ASP     2.5       1     B     369     ASP     2.5       1     B     369     ASP     2.5       1     A     140     VAL     2.5       1     A     140     VAL     2.5       1     A     140     VAL     2.5       1     A     167     ARG     2.4       1     A     333     ASN     2.4       1     A     333     ASN     2.4       1     B     324     LEU     2.4       1     B     327     THR     2.4       1     A     338     SER     2.4  <	Mol	Chain	Res	Type	RSRZ
1     B     370     ILE     2.5       1     B     199     LEU     2.5       1     B     34     GLY     2.5       1     A     196     ASP     2.5       1     B     369     ASP     2.5       1     B     369     ASP     2.5       1     A     140     VAL     2.5       1     A     140     VAL     2.5       1     A     140     VAL     2.5       1     A     167     ARG     2.4       1     A     90     ALA     2.4       1     A     333     ASN     2.4       1     B     324     LEU     2.4       1     B     324     LEU     2.4       1     B     327     THR     2.4       1     B     138     SER     2.4       1     A     373     ARG     2.4 <t< td=""><td></td><td></td><td></td><td></td><td></td></t<>					
1     B     199     LEU     2.5       1     B     34     GLY     2.5       1     A     196     ASP     2.5       1     B     369     ASP     2.5       1     B     87     ALA     2.5       1     A     140     VAL     2.5       1     A     167     ARG     2.4       1     A     90     ALA     2.4       1     A     333     ASN     2.4       1     A     333     ASN     2.4       1     B     324     LEU     2.4       1     B     324     LEU     2.4       1     B     63     ALA     2.4       1     B     327     THR     2.4       1     A     373     ARG     2.4       1     A     197     GLY     2.4       1     A     197     GLY     2.3					
1     B     34     GLY     2.5       1     A     196     ASP     2.5       1     B     369     ASP     2.5       1     B     87     ALA     2.5       1     A     140     VAL     2.5       1     A     167     ARG     2.4       1     A     90     ALA     2.4       1     A     333     ASN     2.4       1     A     333     ASN     2.4       1     B     324     LEU     2.4       1     B     324     LEU     2.4       1     B     327     THR     2.4       1     B     338     SER     2.4       1     B     138     SER     2.4       1     A     197     GLY     2.4       1     A     197     GLY     2.4       1     A     197     GLY     2.3 <tr< td=""><td></td><td></td><td></td><td></td><td></td></tr<>					
1     A     196     ASP     2.5       1     B     369     ASP     2.5       1     B     87     ALA     2.5       1     A     140     VAL     2.5       1     A     167     ARG     2.4       1     A     90     ALA     2.4       1     A     333     ASN     2.4       1     A     333     ASN     2.4       1     B     324     LEU     2.4       1     B     324     LEU     2.4       1     B     327     THR     2.4       1     B     337     THR     2.4       1     A     338     SER     2.4       1     A     338     SER     2.4       1     A     197     GLY     2.4       1     A     197     GLY     2.4       1     A     197     GLY     2.3 <t< td=""><td></td><td></td><td></td><td></td><td></td></t<>					
1     B     369     ASP     2.5       1     B     87     ALA     2.5       1     A     140     VAL     2.5       1     A     167     ARG     2.4       1     A     90     ALA     2.4       1     A     333     ASN     2.4       1     A     333     ASN     2.4       1     B     324     LEU     2.4       1     B     324     LEU     2.4       1     B     327     THR     2.4       1     B     327     THR     2.4       1     A     338     SER     2.4       1     A     373     ARG     2.4       1     A     197     GLY     2.3 <t< td=""><td></td><td></td><td></td><td></td><td></td></t<>					
1     B     87     ALA     2.5       1     A     140     VAL     2.5       1     A     167     ARG     2.4       1     A     90     ALA     2.4       1     A     333     ASN     2.4       1     B     324     LEU     2.4       1     B     324     LEU     2.4       1     B     63     ALA     2.4       1     B     63     ALA     2.4       1     B     324     LEU     2.4       1     B     63     ALA     2.4       1     B     63     ALA     2.4       1     B     327     THR     2.4       1     A     338     SER     2.4       1     A     373     ARG     2.4       1     A     197     GLY     2.4       1     A     197     GLY     2.3					
1     A     140     VAL     2.5       1     A     167     ARG     2.4       1     A     90     ALA     2.4       1     A     333     ASN     2.4       1     B     324     LEU     2.4       1     B     324     LEU     2.4       1     B     327     THR     2.4       1     B     327     THR     2.4       1     B     327     THR     2.4       1     A     338     SER     2.4       1     A     338     SER     2.4       1     A     373     ARG     2.4       1     A     197     GLY     2.4       1     A     197     GLY     2.4       1     A     197     GLY     2.4       1     A     317     VAL     2.3       1     A     326     LEU     2.3  <					
1     A     167     ARG     2.4       1     A     90     ALA     2.4       1     A     333     ASN     2.4       1     B     324     LEU     2.4       1     B     324     LEU     2.4       1     B     63     ALA     2.4       1     B     327     THR     2.4       1     A     338     SER     2.4       1     A     338     SER     2.4       1     A     338     SER     2.4       1     A     373     ARG     2.4       1     A     197     GLY     2.3       1     A     194     ARG     2.3       1     A     194     ARG     2.3 <t< td=""><td></td><td></td><td></td><td></td><td></td></t<>					
1     A     90     ALA     2.4       1     A     333     ASN     2.4       2     E     42     GLY     2.4       1     B     324     LEU     2.4       1     B     63     ALA     2.4       1     B     327     THR     2.4       1     A     338     SER     2.4       1     A     338     SER     2.4       1     A     373     ARG     2.4       1     A     197     GLY     2.3       1     A     326     LEU     2.3       1     A     326     LEU     2.3 <tr< td=""><td></td><td></td><td></td><td></td><td></td></tr<>					
1     A     333     ASN     2.4       2     E     42     GLY     2.4       1     B     324     LEU     2.4       1     B     63     ALA     2.4       1     B     327     THR     2.4       1     A     338     SER     2.4       1     A     338     SER     2.4       1     A     373     ARG     2.4       1     A     197     GLY     2.3       1     A     194     ARG     2.3       1     A     194     ARG     2.3 <t< td=""><td></td><td></td><td></td><td></td><td></td></t<>					
2     E     42     GLY     2.4       1     B     324     LEU     2.4       1     B     63     ALA     2.4       1     B     327     THR     2.4       1     A     338     SER     2.4       1     A     338     SER     2.4       1     A     373     ARG     2.4       1     A     197     GLY     2.3       1     A     326     LEU     2.3       1     A     194     ARG     2.3       1     A     194     ARG     2.3 <t< td=""><td></td><td></td><td></td><td></td><td></td></t<>					
1     B     324     LEU     2.4       1     B     63     ALA     2.4       1     B     327     THR     2.4       1     A     338     SER     2.4       1     B     138     SER     2.4       1     A     373     ARG     2.4       1     A     197     GLY     2.3       1     A     326     LEU     2.3       1     A     194     ARG     2.3       1     A     325     GLY     2.3       2     D     98     HIS     2.3       1     A     105     GLU     2.2 <t< td=""><td></td><td></td><td></td><td></td><td></td></t<>					
1   B   63   ALA   2.4     1   B   327   THR   2.4     1   A   338   SER   2.4     1   B   138   SER   2.4     1   A   373   ARG   2.4     1   A   197   GLY   2.3     1   A   326   LEU   2.3     1   A   194   ARG   2.3     1   A   415   ARG   2.3     1   A   325   GLY   2.3     2   D   98   HIS   2.3     1   A   105   GLU   2.2     1   B   127					
1     B     327     THR     2.4       1     A     338     SER     2.4       1     B     138     SER     2.4       1     A     373     ARG     2.4       1     A     197     GLY     2.3       1     A     326     LEU     2.3       1     A     194     ARG     2.3       1     A     325     GLY     2.3       1     A     325     GLY     2.3       2     D     98     HIS     2.3       1     B     127     THR     2.2  <					
1   A   338   SER   2.4     1   B   138   SER   2.4     1   A   373   ARG   2.4     1   A   197   GLY   2.4     1   A   197   GLY   2.4     1   B   147   VAL   2.3     1   A   81   VAL   2.3     1   A   326   LEU   2.3     1   A   194   ARG   2.3     1   A   194   ARG   2.3     1   A   194   ARG   2.3     1   A   325   GLY   2.3     1   A   325   GLY   2.3     2   D   98   HIS   2.3     1   A   105   GLU   2.2     1   B   127   THR   2.2     1   B   83   LEU   2.2     1   A   411   GLY   2.2     1   B   83 </td <td></td> <td></td> <td></td> <td></td> <td></td>					
1   B   138   SER   2.4     1   A   373   ARG   2.4     1   A   197   GLY   2.4     1   B   147   VAL   2.3     1   A   81   VAL   2.3     1   A   326   LEU   2.3     1   A   194   ARG   2.3     1   A   194   ARG   2.3     1   A   415   ARG   2.3     1   A   325   GLY   2.3     2   D   98   HIS   2.3     1   A   325   GLY   2.3     2   D   98   HIS   2.3     1   A   105   GLU   2.2     2   D   65   LYS   2.2     1   B   127   THR   2.2     1   A   391   LEU   2.2     1   B   83   LEU   2.2     1   B   83 <td></td> <td></td> <td></td> <td></td> <td></td>					
1   A   373   ARG   2.4     1   A   197   GLY   2.4     1   B   147   VAL   2.3     1   A   81   VAL   2.3     1   A   326   LEU   2.3     1   A   194   ARG   2.3     1   A   415   ARG   2.3     1   A   325   GLY   2.3     2   D   98   HIS   2.3     1   A   325   GLY   2.3     2   D   98   HIS   2.3     1   A   105   GLU   2.2     2   D   65   LYS   2.2     1   B   127   THR   2.2     1   A   391   LEU   2.2     1   B   83   LEU   2.2     1   A   411   GLY   2.2     1   B   89   THR   2.2     1   B   335 <td></td> <td></td> <td></td> <td></td> <td></td>					
1   A   197   GLY   2.4     1   B   147   VAL   2.3     1   A   81   VAL   2.3     1   A   326   LEU   2.3     1   A   194   ARG   2.3     1   A   194   ARG   2.3     1   A   415   ARG   2.3     1   A   325   GLY   2.3     2   D   98   HIS   2.3     1   A   325   GLY   2.3     2   D   98   HIS   2.3     1   A   105   GLU   2.2     2   D   65   LYS   2.2     1   B   127   THR   2.2     1   A   391   LEU   2.2     1   B   83   LEU   2.2     1   B   83   LEU   2.2     1   B   89   THR   2.2     1   B   341			138	SER	2.4
1   B   147   VAL   2.3     1   A   81   VAL   2.3     1   A   326   LEU   2.3     1   A   194   ARG   2.3     1   A   415   ARG   2.3     1   A   325   GLY   2.3     2   D   98   HIS   2.3     1   A   105   GLU   2.2     2   D   65   LYS   2.2     1   B   127   THR   2.2     2   E   16   THR   2.2     1   B   83   LEU   2.2     1   B   83   LEU   2.2     1   B   83   LEU   2.2     1   B   85   ILE   2.2     1   B   89   THR   2.2     1   B   341   SER   2.2     1   B   341   SER   2.2     1   A   408	1	A	373		
1   A   81   VAL   2.3     1   A   326   LEU   2.3     1   A   194   ARG   2.3     1   A   415   ARG   2.3     1   A   325   GLY   2.3     2   D   98   HIS   2.3     1   A   105   GLU   2.2     2   D   65   LYS   2.2     1   B   127   THR   2.2     2   E   16   THR   2.2     1   A   391   LEU   2.2     1   B   83   LEU   2.2     1   B   83   LEU   2.2     1   B   255   ILE   2.2     1   B   89   THR   2.2     1   A   378   SER   2.2     1   B   341   SER   2.2     1   B   341   SER   2.2     1   A   408			197	GLY	
1   A   326   LEU   2.3     1   A   194   ARG   2.3     1   A   415   ARG   2.3     1   A   325   GLY   2.3     2   D   98   HIS   2.3     1   A   105   GLU   2.2     2   D   65   LYS   2.2     1   B   127   THR   2.2     2   E   16   THR   2.2     1   A   391   LEU   2.2     1   B   83   LEU   2.2     1   B   83   LEU   2.2     1   B   83   LEU   2.2     1   B   255   ILE   2.2     1   B   89   THR   2.2     1   A   378   SER   2.2     1   B   341   SER   2.2     1   A   408   ARG   2.2     1   A   408	1		147		
1   A   194   ARG   2.3     1   A   415   ARG   2.3     1   A   325   GLY   2.3     2   D   98   HIS   2.3     1   A   105   GLU   2.2     2   D   65   LYS   2.2     1   B   127   THR   2.2     2   E   16   THR   2.2     1   A   391   LEU   2.2     1   B   83   LEU   2.2     1   A   411   GLY   2.2     1   B   255   ILE   2.2     1   B   89   THR   2.2     1   A   378   SER   2.2     1   B   335   ALA   2.2     1   B   341   SER   2.2     1   A   408   ARG   2.2     2   E   67   GLY   2.2	1	A	81	VAL	2.3
1   A   415   ARG   2.3     1   A   325   GLY   2.3     2   D   98   HIS   2.3     1   A   105   GLU   2.2     2   D   65   LYS   2.2     1   B   127   THR   2.2     2   E   16   THR   2.2     1   A   391   LEU   2.2     1   B   83   LEU   2.2     1   A   411   GLY   2.2     1   B   255   ILE   2.2     1   B   89   THR   2.2     1   A   378   SER   2.2     1   B   335   ALA   2.2     1   B   341   SER   2.2     1   A   408   ARG   2.2     2   E   67   GLY   2.2	1		326	LEU	2.3
1   A   325   GLY   2.3     2   D   98   HIS   2.3     1   A   105   GLU   2.2     2   D   65   LYS   2.2     1   B   127   THR   2.2     2   E   16   THR   2.2     1   A   391   LEU   2.2     1   B   83   LEU   2.2     1   A   411   GLY   2.2     1   B   255   ILE   2.2     1   B   89   THR   2.2     1   A   378   SER   2.2     1   B   335   ALA   2.2     1   B   341   SER   2.2     1   A   408   ARG   2.2     2   E   67   GLY   2.2	1	A	194	ARG	2.3
2   D   98   HIS   2.3     1   A   105   GLU   2.2     2   D   65   LYS   2.2     1   B   127   THR   2.2     2   E   16   THR   2.2     1   A   391   LEU   2.2     1   B   83   LEU   2.2     1   A   411   GLY   2.2     1   B   255   ILE   2.2     1   B   89   THR   2.2     1   A   378   SER   2.2     1   B   335   ALA   2.2     1   B   341   SER   2.2     1   A   408   ARG   2.2     2   E   67   GLY   2.2	1	A	415	ARG	2.3
1   A   105   GLU   2.2     2   D   65   LYS   2.2     1   B   127   THR   2.2     2   E   16   THR   2.2     1   A   391   LEU   2.2     1   B   83   LEU   2.2     1   A   411   GLY   2.2     1   B   255   ILE   2.2     1   B   89   THR   2.2     1   A   378   SER   2.2     1   B   335   ALA   2.2     1   B   341   SER   2.2     1   A   408   ARG   2.2     2   E   67   GLY   2.2	1	A	325	GLY	2.3
2   D   65   LYS   2.2     1   B   127   THR   2.2     2   E   16   THR   2.2     1   A   391   LEU   2.2     1   B   83   LEU   2.2     1   A   411   GLY   2.2     1   B   255   ILE   2.2     1   B   89   THR   2.2     1   A   378   SER   2.2     1   B   335   ALA   2.2     1   B   341   SER   2.2     1   A   408   ARG   2.2     2   E   67   GLY   2.2	2	D	98	HIS	2.3
1   B   127   THR   2.2     2   E   16   THR   2.2     1   A   391   LEU   2.2     1   B   83   LEU   2.2     1   A   411   GLY   2.2     1   B   255   ILE   2.2     1   B   89   THR   2.2     1   A   378   SER   2.2     1   B   335   ALA   2.2     1   B   341   SER   2.2     1   A   408   ARG   2.2     2   E   67   GLY   2.2		A	105	l	2.2
2   E   16   THR   2.2     1   A   391   LEU   2.2     1   B   83   LEU   2.2     1   A   411   GLY   2.2     1   B   255   ILE   2.2     1   B   89   THR   2.2     1   A   378   SER   2.2     1   B   335   ALA   2.2     1   B   341   SER   2.2     1   A   408   ARG   2.2     2   E   67   GLY   2.2	2	D	65	LYS	2.2
1   A   391   LEU   2.2     1   B   83   LEU   2.2     1   A   411   GLY   2.2     1   B   255   ILE   2.2     1   B   89   THR   2.2     1   A   378   SER   2.2     1   B   335   ALA   2.2     1   B   341   SER   2.2     1   A   408   ARG   2.2     2   E   67   GLY   2.2	1	В	127	THR	2.2
1 B 83 LEU 2.2   1 A 411 GLY 2.2   1 B 255 ILE 2.2   1 B 89 THR 2.2   1 A 378 SER 2.2   1 B 335 ALA 2.2   1 B 341 SER 2.2   1 A 408 ARG 2.2   2 E 67 GLY 2.2	2	Е	16	THR	2.2
1 B 83 LEU 2.2   1 A 411 GLY 2.2   1 B 255 ILE 2.2   1 B 89 THR 2.2   1 A 378 SER 2.2   1 B 335 ALA 2.2   1 B 341 SER 2.2   1 A 408 ARG 2.2   2 E 67 GLY 2.2	1	A	391	LEU	
1 A 411 GLY 2.2   1 B 255 ILE 2.2   1 B 89 THR 2.2   1 A 378 SER 2.2   1 B 335 ALA 2.2   1 B 341 SER 2.2   1 A 408 ARG 2.2   2 E 67 GLY 2.2	1	В	83	LEU	
1 B 89 THR 2.2   1 A 378 SER 2.2   1 B 335 ALA 2.2   1 B 341 SER 2.2   1 A 408 ARG 2.2   2 E 67 GLY 2.2	1	A	411	GLY	
1   A   378   SER   2.2     1   B   335   ALA   2.2     1   B   341   SER   2.2     1   A   408   ARG   2.2     2   E   67   GLY   2.2	1	В	255	ILE	2.2
1 B 335 ALA 2.2   1 B 341 SER 2.2   1 A 408 ARG 2.2   2 E 67 GLY 2.2	1	В	89	THR	2.2
1 B 341 SER 2.2 1 A 408 ARG 2.2 2 E 67 GLY 2.2	1	A	378	SER	2.2
1 A 408 ARG 2.2 2 E 67 GLY 2.2	1	В	335	ALA	2.2
1 A 408 ARG 2.2 2 E 67 GLY 2.2	1	В	341	SER	2.2
2 E 67 GLY 2.2	1	A		ARG	2.2
	2				
	2	Е	12		2.2



Continued	trom	mromonie	maaa
Continueu	110111	predidus	puyc

Mol	Chain	Res	Type	RSRZ
1	A	193	GLU	2.1
1	В	284	LEU	2.1
1	A	143	ALA	2.1
2	Е	47	VAL	2.1
1	A	100	GLU	2.1
1	A	36	LEU	2.1
1	В	36	LEU	2.1
1	В	167	ARG	2.1
1	В	345	ASP	2.1
1	В	373	ARG	2.1
1	В	90	ALA	2.1
1	В	155	ASN	2.1
1	A	335	ALA	2.1
1	A	342	GLY	2.1
1	В	81	VAL	2.1
1	В	299	LYS	2.1
1	В	285	LEU	2.1
1	A	396	GLN	2.1
1	В	146	PHE	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 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.

