

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

Sep 29, 2022 – 04:22 pm BST

PDB ID	:	8A60
Title	:	Crystal structure of FhuA in complex with the superinfection exclusion
		lipoprotein Llp
Authors	:	van den Berg, B.
Deposited on	:	2022-06-16
Resolution	:	3.37  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)	:	1.13
EDS	:	2.31.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

# 1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.37 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R <sub>free</sub>	130704	1691 (3.46-3.30)
Clashscore	141614	1762 (3.46-3.30)
Ramachandran outliers	138981	1732 (3.46-3.30)
Sidechain outliers	138945	1731 (3.46-3.30)
RSRZ outliers	127900	1635 (3.46-3.30)

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 >=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				
			16%				
1	А	716		70%		22%	• 5%
	-		13%				
2	В	83		47%	27%	• 2	25%



## 2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 5804 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 Ferrichrome outer membrane transporter/phage receptor.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
1	А	677	Total 5307	C 3347	N 897	O 1049	S 14	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	-1	SER	-	expression tag	UNP P06971
А	0	MET	-	expression tag	UNP P06971

• Molecule 2 is a protein called Lytic conversion lipoprotein.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
2	В	62	Total 497	C 324	N 76	O 91	${ m S}{ m 6}$	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
В	63	HIS	-	expression tag	UNP Q38162
В	64	HIS	-	expression tag	UNP Q38162
В	65	HIS	-	expression tag	UNP Q38162
В	66	HIS	-	expression tag	UNP Q38162
В	67	HIS	-	expression tag	UNP Q38162
В	68	HIS	-	expression tag	UNP Q38162



## 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: Ferrichrome outer membrane transporter/phage receptor

• Molecule 2: Lytic conversion lipoprotein





## 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants	98.29Å 98.29Å 236.59Å	Deperitor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $90.00^{\circ}$ $120.00^{\circ}$	Depositor
$\mathbf{P}_{\text{assolution}}(\hat{\mathbf{A}})$	57.85 - 3.37	Depositor
Resolution (A)	85.12 - 3.37	EDS
% Data completeness	77.5 (57.85-3.37)	Depositor
(in resolution range)	78.1 (85.12-3.37)	EDS
$R_{merge}$	(Not available)	Depositor
R <sub>sym</sub>	(Not available)	Depositor
$< I/\sigma(I) > 1$	1.41 (at 3.41 Å)	Xtriage
Refinement program	PHENIX (1.20rc3_4406: ???)	Depositor
B B.	0.253 , $0.307$	Depositor
II, II, <i>free</i>	0.254 , $0.306$	DCC
$R_{free}$ test set	747 reflections $(4.94\%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	95.0	Xtriage
Anisotropy	0.033	Xtriage
Bulk solvent $k_{sol}(e/A^3), B_{sol}(A^2)$	(Not available), (Not available)	EDS
L-test for twinning <sup>2</sup>	$< L >=0.47, < L^2>=0.30$	Xtriage
Estimated twinning fraction	0.043 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.76	EDS
Total number of atoms	5804	wwPDB-VP
Average B, all atoms $(Å^2)$	117.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 2.77% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;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.



<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	Chain	Bond	lengths	Bond angles		
		RMSZ	# Z  > 5	RMSZ	# Z  > 5	
1	А	0.26	0/5438	0.50	0/7387	
2	В	0.26	0/513	0.43	0/692	
All	All	0.26	0/5951	0.50	0/8079	

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	А	5307	0	5036	115	0
2	В	497	0	465	13	0
All	All	5804	0	5501	122	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 11.

All (122) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-1 Atom-2		Clash overlap (Å)
1:A:564:GLU:HG3	1:A:596:THR:HB	1.69	0.74
1:A:429:GLN:HG2	1:A:458:GLN:HG2	1.71	0.71



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:122:ASP:OD2	1:A:199:ARG:NH2	2.24	0.71
1:A:378:VAL:HG12	1:A:434:VAL:HG12	1.74	0.70
1:A:186:ASP:OD1	1:A:187:ASP:N	2.25	0.69
1:A:323:ASN:O	1:A:325:TYR:N	2.28	0.66
1:A:431:GLN:HE22	1:A:502:PRO:HG3	1.61	0.66
1:A:262:LEU:HD21	1:A:402:LEU:HD12	1.78	0.66
1:A:551:ALA:HA	1:A:559:SER:HA	1.79	0.65
1:A:93:ARG:NH2	1:A:520:GLN:OE1	2.30	0.65
1:A:62:GLN:HE21	1:A:709:THR:HG21	1.62	0.64
1:A:178:PHE:CE1	1:A:196:GLY:HA3	2.33	0.64
1:A:329:CYS:O	1:A:337:LYS:NZ	2.30	0.64
1:A:52:VAL:HG22	1:A:130:GLU:HB3	1.81	0.62
1:A:62:GLN:OE1	1:A:679:HIS:NE2	2.31	0.62
1:A:98:GLU:HB2	1:A:103:ASN:HD22	1.66	0.61
1:A:520:GLN:HB2	1:A:543:LEU:HD13	1.83	0.60
1:A:74:PRO:HB3	1:A:587:SER:HB2	1.82	0.59
1:A:599:THR:H	1:A:602:LYS:HD3	1.68	0.59
1:A:598:ASP:O	1:A:600:THR:N	2.36	0.58
1:A:128:ARG:NH1	2:B:42:TYR:O	2.36	0.58
1:A:51:SER:HB3	1:A:133:ARG:HH12	1.69	0.58
1:A:494:PHE:HB3	1:A:523:VAL:HG12	1.85	0.57
1:A:597:THR:HA	1:A:602:LYS:HD2	1.87	0.57
1:A:159:GLU:N	1:A:159:GLU:OE1	2.37	0.57
1:A:496:TYR:OH	1:A:519:LYS:NZ	2.39	0.56
1:A:110:LYS:HZ1	1:A:142:LYS:HD3	1.71	0.55
1:A:98:GLU:OE1	1:A:501:GLU:HB3	2.07	0.55
1:A:637:ARG:NH1	1:A:659:ASP:OD2	2.39	0.55
2:B:14:TYR:HB2	2:B:54:GLU:HG3	1.90	0.54
1:A:98:GLU:H	1:A:103:ASN:N	2.05	0.54
1:A:497:SER:HB2	1:A:520:GLN:HB3	1.90	0.54
1:A:137:SER:O	1:A:479:ARG:NH2	2.41	0.53
1:A:289:GLU:HB2	2:B:19:HIS:ND1	2.24	0.53
1:A:118:ASP:OD1	1:A:118:ASP:N	2.37	0.53
1:A:114:ASN:HD21	1:A:385:ASN:HB2	1.74	0.52
1:A:125:MET:HG3	1:A:234:TYR:HE1	1.75	0.51
1:A:326:SER:HB3	1:A:329:CYS:HB2	1.91	0.51
1:A:74:PRO:HG3	1:A:573:GLU:HB2	1.93	0.51
1:A:295:THR:HB	1:A:362:GLN:HB3	1.93	0.51
1:A:343:ARG:HB2	1:A:397:VAL:HG21	1.93	0.51
1:A:63:PRO:HG2	1:A:69:ALA:HB2	1.92	0.50
2:B:26:VAL:HG22	2:B:36:VAL:HG12	1.92	0.50



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:68:GLU:O	1:A:70:LEU:N	2.45	0.50
1:A:553:PRO:O	1:A:555:GLY:N	2.45	0.50
2:B:39:ILE:HD11	2:B:45:PHE:CE1	2.47	0.49
1:A:92:ILE:HG21	1:A:147:GLY:HA3	1.93	0.49
1:A:599:THR:N	1:A:602:LYS:HB2	2.28	0.49
1:A:447:VAL:HG12	1:A:482:VAL:HG13	1.95	0.48
1:A:95:PHE:CD1	1:A:545:LYS:HE3	2.49	0.48
1:A:327:LYS:N	1:A:395:ASP:OD2	2.47	0.48
1:A:48:GLN:H	2:B:40:MET:HG2	1.79	0.47
1:A:51:SER:OG	1:A:131:ILE:O	2.19	0.47
1:A:423:TYR:CZ	1:A:425:ILE:HG13	2.49	0.47
1:A:98:GLU:HB2	1:A:103:ASN:HA	1.95	0.47
1:A:693:PHE:CZ	1:A:697:GLY:HA3	2.49	0.47
2:B:12:GLU:O	2:B:57:THR:OG1	2.32	0.47
1:A:106:LEU:HG	1:A:107:ASN:HD22	1.79	0.47
1:A:396:SER:HA	1:A:419:ASN:HD22	1.79	0.47
1:A:162:LYS:HB2	1:A:714:PHE:HB2	1.96	0.47
1:A:95:PHE:CG	1:A:545:LYS:HE3	2.50	0.47
1:A:599:THR:OG1	1:A:600:THR:N	2.47	0.47
1:A:71:SER:OG	1:A:637:ARG:HD3	2.16	0.46
1:A:110:LYS:NZ	1:A:142:LYS:HB3	2.30	0.46
1:A:110:LYS:HZ1	1:A:142:LYS:HB3	1.80	0.46
1:A:97:ALA:HB1	1:A:102:GLN:HA	1.97	0.46
1:A:533:PRO:HB3	2:B:37:SER:OG	2.16	0.46
1:A:127:GLU:HB2	1:A:154:LYS:HA	1.97	0.46
1:A:101:SER:OG	1:A:102:GLN:N	2.47	0.46
1:A:102:GLN:OE1	1:A:104:ASN:ND2	2.49	0.46
1:A:69:ALA:C	1:A:71:SER:H	2.19	0.45
1:A:677:ALA:O	1:A:709:THR:N	2.42	0.45
1:A:99:GLY:O	1:A:505:GLN:HG2	2.16	0.45
1:A:145:PRO:HG3	1:A:499:SER:HB3	1.99	0.45
1:A:63:PRO:HB3	1:A:68:GLU:HB2	1.99	0.45
1:A:170:THR:HG22	1:A:706:VAL:H	1.82	0.45
1:A:145:PRO:HD3	1:A:501:GLU:OE1	2.17	0.45
1:A:73:THR:HG21	1:A:131:ILE:HG21	1.98	0.45
1:A:43:ILE:HD13	1:A:530:GLU:HG3	1.99	0.45
2:B:29:ARG:HD3	2:B:62:PHE:CZ	2.52	0.44
1:A:65:SER:N	1:A:68:GLU:OE1	2.48	0.44
1:A:106:LEU:HG	1:A:107:ASN:ND2	2.33	0.44
1:A:48:GLN:O	1:A:50:ILE:HG23	2.18	0.44
1:A:112:GLN:HE21	1:A:119:ALA:HB2	1.83	0.44



	ti a	Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:A:145:PRO:O	1:A:520:GLN:NE2	2.51	0.44	
1:A:255:PRO:HD3	1:A:261:ARG:HH21	1.82	0.44	
1:A:503:SER:OG	1:A:513:PHE:HB2	2.17	0.44	
1:A:40:ASP:O	1:A:41:THR:OG1	2.32	0.44	
1:A:156:PRO:HA	1:A:193:ARG:HB2	1.99	0.43	
1:A:247:LEU:O	1:A:698:CYS:N	2.47	0.43	
1:A:479:ARG:HD3	1:A:497:SER:HA	2.00	0.43	
1:A:397:VAL:HG12	1:A:410:PHE:CE1	2.52	0.43	
1:A:172:SER:O	1:A:172:SER:OG	2.26	0.43	
1:A:43:ILE:HG22	2:B:23:LYS:HB3	2.00	0.43	
2:B:35:LEU:HD13	2:B:46:TRP:CE2	2.53	0.43	
1:A:70:LEU:O	1:A:73:THR:HG22	2.19	0.43	
1:A:453:TYR:CD1	1:A:476:PHE:HB2	2.54	0.43	
1:A:516:SER:OG	1:A:545:LYS:HG2	2.19	0.43	
1:A:49:SER:HB2	2:B:43:GLY:HA2	2.01	0.42	
1:A:501:GLU:H	1:A:501:GLU:HG3	1.61	0.42	
1:A:118:ASP:O	1:A:305:ASN:ND2	2.52	0.42	
1:A:182:ASP:HB3	1:A:192:TYR:HE1	1.85	0.42	
1:A:619:ASP:HA	1:A:633:GLY:HA2	2.02	0.42	
1:A:453:TYR:CE2	1:A:474:LYS:HG2	2.54	0.42	
1:A:52:VAL:HG22	1:A:130:GLU:CB	2.50	0.42	
1:A:527:TYR:CZ	1:A:529:PRO:HG3	2.55	0.42	
1:A:250:GLU:O	1:A:252:THR:N	2.53	0.42	
1:A:73:THR:OG1	1:A:74:PRO:HD2	2.20	0.42	
1:A:140:TYR:O	1:A:479:ARG:NH1	2.52	0.41	
1:A:153:SER:HB2	1:A:232:LEU:HD13	2.01	0.41	
2:B:33:MET:HA	2:B:48:PRO:HA	2.02	0.41	
1:A:483:ASN:HB3	1:A:493:TYR:CB	2.51	0.41	
1:A:115:PHE:HD2	1:A:387:ILE:HG12	1.85	0.41	
1:A:408:THR:HB	1:A:409:ASP:H	1.75	0.41	
1:A:313:TYR:CZ	1:A:344:LYS:HB2	2.56	0.41	
1:A:98:GLU:N	1:A:103:ASN:HB2	2.37	0.40	
1:A:305:ASN:OD1	1:A:306:LYS:N	2.54	0.40	
1:A:54:THR:O	1:A:58:MET:N	2.48	0.40	
1:A:508:LYS:H	1:A:508:LYS:HG2	1.69	0.40	
1:A:663:ARG:HE	1:A:675:ASN:ND2	2.19	0.40	
1:A:70:LEU:CD1	1:A:78:VAL:HG11	2.52	0.40	
1:A:322:ALA:O	1:A:324:ALA:N	2.54	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	А	675/716~(94%)	592 (88%)	67 (10%)	16 (2%)	6 30
2	В	60/83~(72%)	46 (77%)	11 (18%)	3~(5%)	2 15
All	All	735/799~(92%)	638 (87%)	78 (11%)	19 (3%)	5 28

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	А	250	GLU
1	А	49	SER
1	А	69	ALA
1	А	324	ALA
1	А	554	GLU
2	В	56	ASN
1	А	41	THR
1	А	68	GLU
1	А	323	ASN
1	А	407	ASN
1	А	599	THR
1	А	628	SER
1	А	290	PHE
1	А	223	PRO
2	В	31	GLY
1	А	322	ALA
1	А	251	GLY
1	А	398	PRO
2	В	38	PRO

#### 5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent side chain 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.



Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	А	566/593~(95%)	555~(98%)	11 (2%)	57 78
2	В	53/71~(75%)	52~(98%)	1 (2%)	57 78
All	All	619/664~(93%)	607~(98%)	12 (2%)	57 78

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	$\mathbf{Res}$	Type
1	А	70	LEU
1	А	112	GLN
1	А	250	GLU
1	А	260	LYS
1	А	275	TYR
1	А	306	LYS
1	А	315	TYR
1	А	343	ARG
1	А	409	ASP
1	А	550	MET
1	A	612	HIS
2	В	12	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	А	44	GLN
1	А	103	ASN
1	А	431	GLN
2	В	17	GLN

#### 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 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 (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	< <b>RSRZ</b> >	#RSRZ>2		$OWAB(Å^2)$	Q<0.9	
1	А	677/716~(94%)	0.88	117 (17%)	1	<b>2</b>	67, 109, 157, 223	0
2	В	62/83~(74%)	0.99	11 (17%)	1	2	121, 159, 206, 235	0
All	All	739/799~(92%)	0.88	128 (17%)	1	<b>2</b>	67, 112, 171, 235	0

All (128) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	А	246	TRP	9.8
1	А	550	MET	9.7
1	А	557	PHE	9.6
1	А	552	ASP	8.7
1	А	80	THR	8.0
2	В	40	MET	7.3
1	А	81	ARG	7.2
1	А	700	TRP	7.1
1	А	244	TYR	6.6
1	А	699	PHE	6.6
1	А	558	PHE	6.4
1	А	82	GLY	6.4
1	А	551	ALA	6.3
1	А	89	HIS	6.0
1	А	268	GLU	5.9
1	А	48	GLN	5.6
1	А	559	SER	5.5
1	А	44	GLN	5.5
1	А	315	TYR	5.5
1	A	391	PHE	5.4
1	A	267	ASN	5.4
1	А	693	PHE	5.2
1	A	556	SER	5.2
1	A	313	TYR	4.9



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Mol	Chain	Res	Type	RSRZ		
1	А	247	LEU	4.9		
1	А	269	GLY	4.9		
1	А	608	GLN	4.8		
1	А	83	ALA	4.8		
1	А	262	LEU	4.8		
2	В	45	PHE	4.8		
2	В	28	ASP	4.7		
1	А	49	SER	4.7		
1	А	690	ALA	4.7		
2	В	27	PHE	4.6		
1	А	64	LYS	4.5		
1	А	79	GLY	4.4		
1	А	691	SER	4.4		
1	А	47	PRO	4.3		
1	А	689	VAL	4.2		
1	А	116	TYR	4.1		
1	А	74	PRO	4.1		
1	А	78	VAL	4.1		
1	А	90	LEU	4.0		
1	А	88	ASP	4.0		
1	А	50	ILE	4.0		
1	А	314	GLY	3.9		
1	А	696	TYR	3.9		
1	А	95	PHE	3.8		
1	А	101	SER	3.7		
1	А	52	VAL	3.7		
1	А	115	PHE	3.7		
1	А	535	VAL	3.5		
1	А	75	GLY	3.5		
1	А	87	TYR	3.5		
1	А	688	TYR	3.5		
1	А	652	VAL	3.4		
1	А	509	ASP	3.4		
1	А	698	CYS	3.3		
1	А	606	PRO	3.3		
1	А	701	GLY	3.3		
1	А	643	TYR	3.2		
1	А	245	GLY	3.2		
1	А	705	GLN	3.2		
1	А	573	GLU	3.2		
1	А	252	THR	3.2		
1	А	91	ILE	3.1		



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Mol	Chain	Res	Type	RSRZ
1	А	248	PRO	3.1
1	А	84	SER	3.1
1	А	85	ASN	3.1
1	А	102	GLN	3.1
1	А	536	VAL	3.1
2	В	10	LYS	3.1
1	А	266	PHE	3.0
1	А	610	PRO	3.0
1	А	513	PHE	3.0
1	А	575	LYS	3.0
1	А	651	LYS	3.0
2	В	46	TRP	2.9
1	А	407	ASN	2.9
1	А	508	LYS	2.9
1	А	46	VAL	2.9
1	А	571	GLU	2.8
1	А	528	VAL	2.8
1	А	588	TYR	2.8
1	А	249	LYS	2.7
1	А	644	GLY	2.7
1	А	133	ARG	2.7
1	А	100	GLN	2.7
1	А	94	GLY	2.6
1	А	650	PHE	2.6
1	А	73	THR	2.6
1	А	128	ARG	2.6
1	А	312	VAL	2.6
1	А	505	GLN	2.6
1	А	534	ILE	2.6
1	А	45	LYS	2.6
2	В	38	PRO	2.6
1	А	423	TYR	2.6
1	А	605	THR	2.6
1	А	77	SER	2.5
1	А	70	LEU	2.5
1	А	568	ARG	2.5
1	А	607	ALA	2.4
1	А	555	GLY	2.4
1	А	592	ASP	2.4
1	А	341	LEU	2.4
2	В	36	VAL	2.4
1	А	554	GLU	2.4



Mol	Chain	Res	Type	RSRZ
1	А	609	VAL	2.4
1	А	175	GLN	2.4
1	А	560	VAL	2.3
1	А	714	PHE	2.3
2	В	39	ILE	2.3
1	А	66	VAL	2.3
1	А	590	TYR	2.3
1	А	611	LYS	2.2
1	А	533	PRO	2.2
2	В	30	LYS	2.2
1	А	93	ARG	2.2
1	А	574	ALA	2.1
1	А	511	ASN	2.1
1	А	697	GLY	2.1
1	А	358	ASP	2.1
2	В	17	GLN	2.1
1	А	111	LEU	2.1
1	А	174	PHE	2.0
1	А	645	ASP	2.1
1	А	166	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.

