

Full wwPDB X-ray Structure Validation Report (i)

May 23, 2022 – 01:14 pm BST

PDB ID	:	70HZ
Title	:	Crystal structure of AP2 Mu2 - FCHO2 chimera (His6-tagged)
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Deposited on	:	2021-05-11
Resolution	:	2.27 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 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	:	2.28.1
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)	:	2.28.1

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 2.27 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 $(\text{\AA}))$
R _{free}	130704	6980 (2.30-2.26)
Clashscore	141614	7711 (2.30-2.26)
Ramachandran outliers	138981	7597 (2.30-2.26)
Sidechain outliers	138945	7598 (2.30-2.26)
RSRZ outliers	127900	6849 (2.30-2.26)

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				
			36%				
1	А	361	69%	9%	•	21%	
			38%				
1	В	361	66%	12%	•	21%	



2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 4761 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.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
1	В	285	Total	\mathbf{C}	Ν	Ο	\mathbf{S}	0	Ο	Ο
1	D	200	2307	1475	409	409	14	0	0	0
1	Δ	285	Total	С	Ν	0	S	0	0	0
	1 A	200	2309	1476	410	409	14	0	0	0

• Molecule 1 is a protein called AP-2 complex subunit mu,F-BAR domain only protein 2.

Chain	Residue	Modelled	Actual Comment		Reference
В	151	MET	-	initiating methionine	UNP P84092
В	152	HIS	-	expression tag	UNP P84092
В	153	HIS	-	expression tag	UNP P84092
В	154	HIS	-	expression tag	UNP P84092
В	155	HIS	-	expression tag	UNP P84092
В	156	HIS	-	expression tag	UNP P84092
В	157	HIS	-	expression tag	UNP P84092
В	436	GLY	-	linker	UNP P84092
В	437	ALA	-	linker	UNP P84092
В	438	SER	-	linker	UNP P84092
В	439	GLY	-	linker	UNP P84092
В	440	SER	-	linker	UNP P84092
В	441	ALA	-	linker	UNP P84092
В	442	GLY	-	linker	UNP P84092
В	443	SER	-	linker	UNP P84092
В	444	ALA	-	linker	UNP P84092
В	445	GLY	-	linker	UNP P84092
В	446	PRO	-	linker	UNP P84092
В	447	SER	-	linker	UNP P84092
В	448	GLY	-	linker	UNP P84092
В	449	ALA	-	linker	UNP P84092
В	450	GLY	-	linker	UNP P84092
В	451	SER	-	linker	UNP P84092
В	452	ALA	-	linker	UNP P84092
В	453	GLY	-	linker	UNP P84092

There are 94 discrepancies between the modelled and reference sequences:



Chain	Residue	Modelled	Actual	Comment	Reference
В	454	SER	-	linker	UNP P84092
В	455	ALA	-	linker	UNP P84092
В	456	GLY	-	linker	UNP P84092
В	457	PRO	-	linker	UNP P84092
В	458	SER	_	linker	UNP P84092
В	459	ALA	_	linker	UNP P84092
В	460	GLY	_	linker	UNP P84092
В	461	SER	-	linker	UNP P84092
В	462	ALA	-	linker	UNP P84092
В	463	GLY	-	linker	UNP P84092
В	464	SER	-	linker	UNP P84092
В	465	ALA	-	linker	UNP P84092
В	466	GLY	-	linker	UNP P84092
В	467	SER	-	linker	UNP P84092
В	468	GLY	-	linker	UNP P84092
В	469	SER	-	linker	UNP P84092
В	470	ALA	-	linker	UNP P84092
В	471	GLY	-	linker	UNP P84092
В	472	SER	-	linker	UNP P84092
В	473	ALA	-	linker	UNP P84092
В	474	PRO	-	linker	UNP P84092
В	475	GLY	-	linker	UNP P84092
А	151	MET	-	initiating methionine	UNP P84092
А	152	HIS	-	expression tag	UNP P84092
A	153	HIS	-	expression tag	UNP P84092
А	154	HIS	-	expression tag	UNP P84092
А	155	HIS	-	expression tag	UNP P84092
A	156	HIS	-	expression tag	UNP P84092
A	157	HIS	-	expression tag	UNP P84092
A	436	GLY	-	linker	UNP P84092
A	437	ALA	-	linker	UNP P84092
A	438	SER	-	linker	UNP P84092
A	439	GLY	-	linker	UNP P84092
A	440	SER	-	linker	UNP P84092
A	441	ALA	-	linker	UNP P84092
A	442	GLY	-	linker	UNP P84092
A	443	SER	-	linker	UNP P84092
A	444	ALA	-	linker	UNP P84092
A	445	GLY	-	linker	UNP P84092
A	446	PRO	-	linker	UNP P84092
A	447	SER	-	linker	UNP P84092
A A	448	GLY	-	linker	UNP P84092



Chain	Residue	Modelled	Actual	Comment	Reference
А	449	ALA	-	linker	UNP P84092
А	450	GLY	-	linker	UNP P84092
А	451	SER	-	linker	UNP P84092
А	452	ALA	-	linker	UNP P84092
А	453	GLY	-	linker	UNP P84092
А	454	SER	_	linker	UNP P84092
А	455	ALA	_	linker	UNP P84092
А	456	GLY	_	linker	UNP P84092
А	457	PRO	-	linker	UNP P84092
А	458	SER	-	linker	UNP P84092
А	459	ALA	-	linker	UNP P84092
А	460	GLY	-	linker	UNP P84092
А	461	SER	-	linker	UNP P84092
А	462	ALA	-	linker	UNP P84092
А	463	GLY	-	linker	UNP P84092
А	464	SER	-	linker	UNP P84092
А	465	ALA	-	linker	UNP P84092
А	466	GLY	-	linker	UNP P84092
А	467	SER	-	linker	UNP P84092
А	468	GLY	-	linker	UNP P84092
А	469	SER	-	linker	UNP P84092
А	470	ALA	-	linker	UNP P84092
А	471	GLY	-	linker	UNP P84092
А	472	SER	-	linker	UNP P84092
А	473	ALA	-	linker	UNP P84092
А	474	PRO	-	linker	UNP P84092
А	475	GLY	_	linker	UNP P84092

• Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	В	62	TotalO6262	0	0
2	А	83	Total O 83 83	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: AP-2 complex subunit mu,F-BAR domain only protein 2

SER ASP SER ASP GLU GLU GLU

• Molecule 1: AP-2 complex subunit mu,F-BAR domain only protein 2





ALA 1386 ALA 1386 ALA 1386 ALA F390 SER F390 SER F390 SER F390 SER F390 SER F390 GLY F300 SER F300 GLY F303 SER F304 GLY F405 GLY F405 PAT F413 </tr



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	55.68Å 129.86Å 64.42 Å	Deperitor
a, b, c, α , β , γ	90.00° 102.47° 90.00°	Depositor
$\mathbf{P}_{\text{oscolution}}(\hat{\mathbf{A}})$	62.90 - 2.27	Depositor
Resolution (A)	62.90 - 2.27	EDS
% Data completeness	95.9 (62.90-2.27)	Depositor
(in resolution range)	97.0 (62.90-2.27)	EDS
R_{merge}	0.14	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	1.77 (at 2.27Å)	Xtriage
Refinement program	REFMAC 5.8.0257, PHENIX 1.19rc1_4016	Depositor
P. P.	0.267 , 0.314	Depositor
Λ, Λ_{free}	0.270 , 0.316	DCC
R_{free} test set	1989 reflections (4.96%)	wwPDB-VP
Wilson B-factor $(Å^2)$	38.1	Xtriage
Anisotropy	0.698	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	(Not available), (Not available)	EDS
L-test for $twinning^2$	$ L > = 0.48, < L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	4761	wwPDB-VP
Average B, all atoms $(Å^2)$	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The analyses of the Patterson function reveals a significant off-origin peak that is 32.09 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 9.9390e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.

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.



¹Intensities 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		
	Ullaili	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.29	0/2361	0.54	0/3175	
1	В	0.25	0/2359	0.53	0/3173	
All	All	0.27	0/4720	0.54	0/6348	

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	2309	0	2347	27	0
1	В	2307	0	2346	30	0
2	А	83	0	0	0	0
2	В	62	0	0	0	0
All	All	4761	0	4693	56	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 6.

All (56) 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:333:VAL:HG11	1:A:370:ILE:HG13	1.28	1.13



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:333:VAL:HG12	1:A:370:ILE:HA	1.05	1.05
1:A:333:VAL:CG1	1:A:370:ILE:HG13	1.92	0.98
1:A:333:VAL:CG1	1:A:370:ILE:HA	1.96	0.95
1:A:333:VAL:HG12	1:A:370:ILE:CA	1.97	0.92
1:A:345:LYS:HE3	1:A:352:VAL:HB	1.67	0.77
1:B:392:VAL:HG13	1:B:394:PHE:CE2	2.25	0.71
1:B:218:ASP:OD1	1:B:219:LYS:NZ	2.27	0.68
1:B:479:ASP:HB3	1:B:485:ILE:HD11	1.77	0.65
1:A:301:LEU:HB2	1:A:370:ILE:HB	1.79	0.65
1:A:479:ASP:HB3	1:A:485:ILE:HD11	1.79	0.63
1:B:392:VAL:CG1	1:B:394:PHE:CE2	2.83	0.62
1:B:196:VAL:HG23	1:B:283:ILE:HD13	1.82	0.62
1:B:383:ARG:HB2	1:B:437:ALA:HB3	1.82	0.61
1:A:327:PRO:HD2	1:A:330:THR:CG2	2.33	0.58
1:B:213:LYS:HG2	1:B:403:TYR:HE1	1.69	0.58
1:B:278:ARG:NH2	1:A:192:LEU:O	2.36	0.58
1:A:306:VAL:HG22	1:A:365:GLN:HG2	1.84	0.57
1:A:176:ASP:HB3	1:A:178:LEU:HD21	1.84	0.57
1:A:333:VAL:HG11	1:A:370:ILE:CG1	2.19	0.56
1:B:392:VAL:HG11	1:B:394:PHE:CZ	2.41	0.56
1:A:296:VAL:HB	1:A:300:LYS:HB2	1.90	0.54
1:B:392:VAL:HG13	1:B:394:PHE:CD2	2.44	0.53
1:B:250:GLN:H	1:B:250:GLN:CD	2.13	0.51
1:B:175:LEU:HD11	1:B:404:LEU:HD22	1.92	0.51
1:B:293:VAL:HG12	1:B:303:VAL:HG22	1.93	0.50
1:A:174:PHE:HB2	1:A:203:LYS:HB2	1.94	0.49
1:A:307:ILE:HG13	1:A:364:SER:O	2.12	0.49
1:B:392:VAL:HG12	1:B:394:PHE:H	1.79	0.48
1:B:241:ILE:HD12	1:B:399:LEU:HB2	1.96	0.48
1:B:167:LYS:HB3	1:B:483:TYR:CD1	2.49	0.48
1:B:399:LEU:HD23	1:B:400:LYS:N	2.29	0.47
1:A:159:ILE:HG22	1:A:162:ARG:H	1.79	0.47
1:A:333:VAL:CG1	1:A:370:ILE:CG1	2.79	0.47
1:B:216:MET:HG2	1:B:399:LEU:HD21	1.97	0.46
1:A:327:PRO:HD2	1:A:330:THR:HG22	1.97	0.46
1:B:392:VAL:CG1	1:B:394:PHE:CD2	2.99	0.45
1:B:303:VAL:HB	1:B:368:ALA:HB3	1.98	0.45
1:A:333:VAL:HG12	1:A:370:ILE:HG13	1.89	0.45
1:A:403:TYR:CD1	1:A:405:LYS:HG2	2.51	0.45
1:A:159:ILE:HG23	1:A:161:TRP:CD2	2.53	0.44
1:B:203:LYS:HG2	1:B:271:GLU:HG3	1.99	0.44



Atom-1	Atom-2	Interatomic distance $(Å)$	Clash
	1. A. OCT. OI N.CO		
1:A:300:VAL:HG22	1:A:305:GLN:CG	2.48	0.43
1:B:410:LYS:HE3	1:B:410:LYS:HB3	1.90	0.43
1:B:485:ILE:N	1:B:485:ILE:HD13	2.34	0.42
1:B:293:VAL:HG12	1:B:303:VAL:HG13	2.01	0.42
1:A:291:PRO:HB3	1:A:305:VAL:HG22	2.03	0.41
1:A:327:PRO:HD2	1:A:330:THR:HG21	2.00	0.41
1:B:168:TYR:CE1	1:B:484:SER:HB2	2.56	0.41
1:B:162:ARG:HD2	1:B:267:PRO:O	2.20	0.41
1:B:484:SER:C	1:B:485:ILE:HD13	2.41	0.41
1:A:308:LYS:HG2	1:A:363:GLU:HG2	2.02	0.40
1:B:353:TRP:CE2	1:B:355:ILE:HD11	2.57	0.40
1:A:245:ASP:N	1:A:245:ASP:OD1	2.54	0.40
1:B:325:PRO:HG3	1:B:384:PRO:O	2.22	0.40
1:B:389:ASN:HA	1:B:428:SER:OG	2.21	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	277/361 (77%)	259~(94%)	16~(6%)	2(1%)	22 25
1	В	277/361~(77%)	262~(95%)	15~(5%)	0	100 100
All	All	554/722~(77%)	521 (94%)	31(6%)	2(0%)	34 40

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	А	153	HIS
1	А	291	PRO



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 side chain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	А	258/307~(84%)	251~(97%)	7 (3%)	44 59
1	В	258/307~(84%)	247~(96%)	11 (4%)	29 38
All	All	516/614~(84%)	498 (96%)	18 (4%)	36 48

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	В	156	HIS
1	В	169	ARG
1	В	176	ASP
1	В	219	LYS
1	В	250	GLN
1	В	262	SER
1	В	314	SER
1	В	333	VAL
1	В	402	ARG
1	В	408	GLU
1	В	410	LYS
1	А	152	HIS
1	А	156	HIS
1	А	314	SER
1	А	364	SER
1	А	365	GLN
1	А	408	GLU
1	А	414	SER

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

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	<RSRZ $>$	#RSRZ>2		$OWAB(Å^2)$	Q<0.9
1	А	285/361~(78%)	2.21	130~(45%) 0	0	22, 48, 90, 135	0
1	В	285/361~(78%)	2.21	138 (48%) 0	0	22, 49, 85, 119	0
All	All	570/722~(78%)	2.21	268 (47%) 0	0	22, 49, 88, 135	0

All (268) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	А	328	LEU	11.6
1	А	377	ASP	10.6
1	В	351	ILE	10.2
1	В	343	LYS	8.9
1	А	352	VAL	8.0
1	А	342	ALA	7.5
1	А	351	ILE	7.3
1	В	324	ILE	6.9
1	А	374	PRO	6.7
1	В	186	SER	6.7
1	А	343	LYS	6.6
1	В	477	ASP	6.5
1	А	157	HIS	6.3
1	В	301	LEU	6.1
1	В	157	HIS	6.0
1	А	324	ILE	5.8
1	В	328	LEU	5.8
1	А	376	ASN	5.7
1	В	338	MET	5.7
1	В	376	ASN	5.6
1	В	342	ALA	5.6
1	В	352	VAL	5.5
1	В	435	CYS	5.5
1	В	378	LYS	5.5



Mol	Chain	Res	Type	RSRZ
1	А	152	HIS	5.4
1	В	241	ILE	5.2
1	А	370	ILE	5.2
1	А	333	VAL	5.1
1	А	381	TRP	5.1
1	А	436	GLY	5.1
1	В	489	THR	5.0
1	А	336	ILE	5.0
1	А	478	VAL	5.0
1	А	301	LEU	5.0
1	В	377	ASP	4.8
1	А	335	VAL	4.8
1	А	293	VAL	4.7
1	В	208	GLY	4.7
1	А	298	ARG	4.5
1	А	502	SER	4.5
1	А	327	PRO	4.4
1	В	154	HIS	4.4
1	В	322	VAL	4.4
1	В	161	TRP	4.3
1	А	154	HIS	4.3
1	В	374	PRO	4.3
1	А	435	CYS	4.3
1	А	338	MET	4.1
1	В	434	ARG	4.1
1	В	206	LEU	4.1
1	А	175	LEU	4.1
1	А	353	TRP	4.0
1	В	169	ARG	4.0
1	В	430	ILE	4.0
1	A	193	SER	4.0
1	В	372	LEU	3.9
1	A	202	MET	3.9
1	А	433	THR	3.9
1	В	298	ARG	3.8
1	A	206	LEU	3.8
1	В	254	LEU	3.8
1	В	478	VAL	3.8
1	В	216	MET	3.8
1	А	332	GLY	3.7
1	В	262	SER	3.7
1	А	165	GLY	3.6



Mol	Chain	Res	Type	RSRZ
1	В	268	PRO	3.6
1	А	344	TYR	3.6
1	А	180	SER	3.6
1	А	380	LYS	3.5
1	А	208	GLY	3.5
1	В	292	LEU	3.5
1	В	357	ARG	3.5
1	В	380	LYS	3.5
1	А	407	PHE	3.5
1	А	246	CYS	3.5
1	А	434	ARG	3.5
1	В	296	VAL	3.4
1	В	202	MET	3.4
1	A	316	LEU	3.4
1	А	322	VAL	3.4
1	А	414	SER	3.4
1	В	293	VAL	3.4
1	В	361	MET	3.4
1	В	333	VAL	3.3
1	В	153	HIS	3.3
1	А	367	SER	3.3
1	В	289	VAL	3.3
1	А	350	ALA	3.3
1	А	477	ASP	3.3
1	В	280	THR	3.3
1	А	375	THR	3.3
1	А	365	GLN	3.2
1	А	418	VAL	3.2
1	В	218	ASP	3.2
1	А	209	MET	3.2
1	В	360	GLY	3.2
1	А	386	ILE	3.2
1	В	381	TRP	3.2
1	A	171	ASN	3.2
1	A	161	TRP	3.1
1	А	421	TRP	3.1
1	В	326	THR	3.1
1	A	259	SER	3.1
1	В	247	THR	3.1
1	A	306	VAL	3.1
1	В	433	THR	3.1
1	В	407	PHE	3.0



Mol	Chain	Res	Type	RSRZ
1	В	269	ASP	3.0
1	В	323	ARG	3.0
1	В	365	GLN	3.0
1	А	323	ARG	3.0
1	В	193	SER	3.0
1	А	272	PHE	3.0
1	В	173	LEU	3.0
1	А	406	VAL	3.0
1	В	266	ILE	2.9
1	В	413	TYR	2.9
1	А	194	ALA	2.9
1	В	191	VAL	2.9
1	В	314	SER	2.9
1	В	184	LEU	2.9
1	А	404	LEU	2.9
1	В	214	PHE	2.8
1	А	420	LYS	2.8
1	В	411	LEU	2.8
1	В	483	TYR	2.8
1	А	355	ILE	2.8
1	А	188	GLN	2.8
1	В	210	PRO	2.8
1	А	195	HIS	2.8
1	В	260	GLU	2.8
1	В	243	ILE	2.8
1	А	266	ILE	2.8
1	В	424	TYR	2.8
1	А	218	ASP	2.7
1	В	500	TYR	2.7
1	В	498	HIS	2.7
1	В	386	ILE	2.7
1	A	177	VAL	2.7
1	А	173	LEU	2.7
1	В	482	GLY	2.7
1	В	319	LYS	2.7
1	A	357	ARG	2.7
1	В	315	LEU	2.7
1	А	274	LEU	2.7
1	В	283	ILE	2.7
1	А	307	ILE	2.7
1	В	394	PHE	2.7
1	В	310	ASN	2.6



Mol	Chain	Res	Type	RSRZ
1	В	178	LEU	2.6
1	В	311	PHE	2.6
1	А	311	PHE	2.6
1	В	416	HIS	2.6
1	А	178	LEU	2.6
1	А	289	VAL	2.6
1	А	268	PRO	2.6
1	В	375	THR	2.6
1	В	258	ASP	2.6
1	В	502	SER	2.6
1	А	315	LEU	2.6
1	А	159	ILE	2.6
1	А	186	SER	2.6
1	A	347	SER	2.6
1	А	500	TYR	2.6
1	А	425	ILE	2.6
1	В	175	LEU	2.6
1	В	195	HIS	2.6
1	А	190	GLN	2.6
1	В	404	LEU	2.5
1	В	257	PHE	2.5
1	А	359	ALA	2.5
1	В	320	ILE	2.5
1	А	326	THR	2.5
1	В	304	LYS	2.5
1	В	399	LEU	2.5
1	А	303	VAL	2.5
1	А	371	GLU	2.5
1	А	158	GLN	2.5
1	В	436	GLY	2.5
1	В	300	LYS	2.5
1	В	364	SER	2.5
1	В	406	VAL	2.5
1	А	413	TYR	2.5
1	В	240	SER	2.4
1	В	317	ALA	2.4
1	В	390	PHE	2.4
1	А	399	LEU	2.4
1	В	405	LYS	2.4
1	В	385	PRO	2.4
1	А	184	LEU	2.4
1	А	331	SER	2.4



Mol	Chain	Res	Type	RSRZ
1	В	358	MET	2.4
1	А	275	MET	2.4
1	В	174	PHE	2.4
1	В	418	VAL	2.4
1	В	251	CYS	2.4
1	А	424	TYR	2.4
1	В	353	TRP	2.4
1	В	402	ARG	2.4
1	В	156	HIS	2.4
1	А	317	ALA	2.4
1	А	368	ALA	2.4
1	В	158	GLN	2.4
1	В	316	LEU	2.3
1	В	363	GLU	2.3
1	А	192	LEU	2.3
1	А	183	LEU	2.3
1	А	349	ASN	2.3
1	А	212	CYS	2.3
1	А	210	PRO	2.3
1	В	159	ILE	2.3
1	В	166	ILE	2.3
1	В	274	LEU	2.3
1	А	362	LYS	2.3
1	В	188	GLN	2.3
1	В	200	VAL	2.3
1	А	304	LYS	2.3
1	А	411	LEU	2.3
1	А	155	HIS	2.3
1	А	310	ASN	2.3
1	В	313	PRO	2.3
1	В	305	VAL	2.2
1	А	314	SER	2.2
1	В	354	LYS	2.2
1	A	360	GLY	2.2
1	A	426	GLY	2.2
1	А	153	HIS	2.2
1	В	291	PRO	2.2
1	В	303	VAL	2.2
1	В	306	VAL	2.2
1	A	305	VAL	2.2
1	В	501	SER	2.2
1	В	307	ILE	2.2



Mol	Chain	Res	Type	RSRZ
1	В	485	ILE	2.2
1	В	270	GLY	2.2
1	А	299	THR	2.2
1	А	366	ILE	2.2
1	В	318	GLN	2.2
1	А	390	PHE	2.1
1	В	488	GLU	2.1
1	А	176	ASP	2.1
1	А	249	HIS	2.1
1	В	252	VAL	2.1
1	В	392	VAL	2.1
1	А	172	GLU	2.1
1	В	415	ASP	2.1
1	А	269	ASP	2.1
1	А	396	PRO	2.1
1	А	430	ILE	2.1
1	В	287	PHE	2.1
1	А	402	ARG	2.1
1	А	241	ILE	2.1
1	В	302	GLU	2.1
1	В	368	ALA	2.1
1	А	382	ALA	2.1
1	А	422	VAL	2.1
1	В	272	PHE	2.1
1	А	302	GLU	2.0
1	В	171	ASN	2.0
1	В	412	ASN	2.0
1	А	403	TYR	2.0
1	В	263	ILE	2.0
1	А	346	ALA	2.0
1	А	417	ASP	2.0
1	В	401	VAL	2.0
1	А	205	TYR	2.0
1	В	264	SER	2.0

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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.

