

Full wwPDB X-ray Structure Validation Report (i)

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PDB ID	:	8C7T
Title	:	Unliganded transcriptional pleiotropic repressor CodY from Enterococcus fae-
		calis
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Deposited on	:	2023-01-17
Resolution	:	2.21 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	:	2.35
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)	:	2.35

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 2.21 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	Similar resolution		
	$(\# { m Entries})$	$(\# { m Entries}, { m resolution} { m range}({ m \AA}))$		
R_{free}	130704	5912 (2.24-2.20)		
Clashscore	141614	6646 (2.24-2.20)		
Ramachandran outliers	138981	6543 (2.24-2.20)		
Sidechain outliers	138945	6544 (2.24-2.20)		
RSRZ outliers	127900	5797 (2.24-2.20)		

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		000	16%					
	A	262			87%			13%
			29%					
1	В	262			82%			18%
			8%					
1	С	262		56%		12%	32%	
			21%					
1	D	262			87%			13%



2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 7659 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		At	oms			ZeroOcc	AltConf	Trace
1	Δ	261	Total	С	Ν	0	\mathbf{S}	0	0	0
	A	201	2031	1290	336	397	8	0	0	U
1	р	262	Total	С	Ν	0	S	0	1	0
1	ГБ	202	2048	1301	339	400	8	0	1	0
1	C	170	Total	С	Ν	0	S	0	0	0
		178	1398	893	228	270	7	0	0	0
1 D	262	Total	С	Ν	0	S	0	0	0	
	202	2041	1296	338	399	8	0	U	U	

• Molecule 1 is a protein called GTP-sensing transcriptional pleiotropic repressor CodY.

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	-1	GLY	-	expression tag	UNP A0A1B4XP18
А	0	ALA	-	expression tag	UNP A0A1B4XP18
В	-1	GLY	-	expression tag	UNP A0A1B4XP18
В	0	ALA	-	expression tag	UNP A0A1B4XP18
С	-1	GLY	-	expression tag	UNP A0A1B4XP18
С	0	ALA	-	expression tag	UNP A0A1B4XP18
D	-1	GLY	-	expression tag	UNP A0A1B4XP18
D	0	ALA	-	expression tag	UNP A0A1B4XP18

• Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	А	12	Total O 12 12	0	0
2	В	53	Total O 53 53	0	0
2	С	21	Total O 21 21	0	0
2	D	55	$\begin{array}{cc} {\rm Total} & {\rm O} \\ 55 & 55 \end{array}$	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: GTP-sensing transcriptional pleiotropic repressor CodY



• Molecule 1: GTP-sensing transcriptional pleiotropic repressor CodY





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	32.99Å 171.24Å 215.24Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Bosolution (Å)	35.87 - 2.21	Depositor
Resolution (A)	35.87 - 2.21	EDS
% Data completeness	99.8 (35.87-2.21)	Depositor
(in resolution range)	99.8 (35.87-2.21)	EDS
R _{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.49 (at 2.22 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
P. P.	0.236 , 0.273	Depositor
n, n_{free}	0.241 , 0.274	DCC
R_{free} test set	3191 reflections $(5.09%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	41.9	Xtriage
Anisotropy	0.371	Xtriage
Bulk solvent $k_{sol}(e/A^3)$, $B_{sol}(A^2)$	0.29 , 42.8	EDS
L-test for $twinning^2$	$ < L >=0.49, < L^2>=0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	7659	wwPDB-VP
Average B, all atoms $(Å^2)$	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.91% of the height of the origin peak. No significant pseudotranslation is detected.

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).

Mal	Chain	Bond	lengths	Bond angles	
		RMSZ	# Z > 5	RMSZ	# Z > 5
1	А	0.52	0/2057	0.68	0/2777
1	В	0.60	0/2074	0.75	0/2798
1	С	0.55	0/1418	0.63	0/1916
1	D	0.64	0/2067	0.71	0/2788
All	All	0.58	0/7616	0.70	0/10279

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	2031	0	2076	19	0
1	В	2048	0	2097	29	0
1	С	1398	0	1424	23	0
1	D	2041	0	2089	21	0
2	А	12	0	0	0	0
2	В	53	0	0	0	0
2	С	21	0	0	0	0
2	D	55	0	0	0	0
All	All	7659	0	7686	84	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.



A 1 A		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:202:GLU:O	1:B:249:VAL:HG23	1.81	0.81
1:C:157:MET:HE3	1:D:160:LEU:HD12	1.62	0.80
1:C:157:MET:CE	1:D:160:LEU:HD12	2.13	0.78
1:B:188:GLU:HB3	1:B:225:ALA:HB2	1.68	0.75
1:B:22:ASP:CG	1:B:25:ALA:HB2	2.14	0.68
1:B:187:SER:HB3	1:B:221:VAL:HG11	1.76	0.68
1:D:205:ARG:O	1:D:206:LEU:HD12	1.94	0.66
1:C:39:ILE:HG22	1:C:147:LEU:HD21	1.77	0.65
1:D:198:ALA:HB3	1:D:206:LEU:HD21	1.81	0.63
1:B:187:SER:HB3	1:B:221:VAL:CG1	2.29	0.63
1:A:254:PHE:HE1	1:A:258:LEU:HD22	1.64	0.63
1:B:188:GLU:OE1	1:B:224:ASN:ND2	2.32	0.62
1:B:27:LEU:HB3	1:B:54:LEU:O	2.01	0.60
1:A:190:LYS:HE3	1:A:215:ILE:HD11	1.85	0.57
1:D:4:LEU:O	1:D:8:THR:HG23	2.05	0.57
1:A:131:ILE:HD11	1:A:155:VAL:HG21	1.86	0.56
1:A:178:GLN:NE2	1:A:257:GLU:OE1	2.38	0.56
1:D:175:THR:HA	1:D:178:GLN:OE1	2.05	0.56
1:D:135:ARG:HG3	1:D:140:PHE:CZ	2.41	0.56
1:B:29:TYR:CD1	1:B:32:MET:HE2	2.41	0.55
1:C:36:LEU:HD11	1:C:155:VAL:HG21	1.88	0.55
1:D:254:PHE:HE1	1:D:258:LEU:HD22	1.71	0.55
1:A:121:LEU:HD23	1:A:152:ALA:HB1	1.89	0.54
1:B:199:LEU:HD11	1:B:204:GLY:CA	2.38	0.54
1:B:188:GLU:O	1:B:192:VAL:HG23	2.07	0.54
1:B:188:GLU:O	1:B:191:ALA:HB3	2.07	0.53
1:A:27:LEU:HB3	1:A:54:LEU:O	2.09	0.53
1:A:87:LEU:HD12	1:A:87:LEU:N	2.24	0.52
1:C:175:THR:O	1:C:179:MET:HG2	2.09	0.52
1:B:240:LEU:HD11	1:B:246:TYR:HB2	1.91	0.51
1:B:24:GLN:HG3	1:B:24:GLN:O	2.11	0.50
1:D:199:LEU:HD11	1:D:204:GLY:N	2.27	0.50
1:B:166:THR:HG22	1:B:170:GLU:HG3	1.94	0.50
1:A:4:LEU:O	1:A:8:THR:HG23	2.13	0.49
1:C:107:SER:O	1:C:107:SER:OG	2.26	0.49
1:B:164:SER:O	1:B:167:ILE:HG22	2.13	0.48
1:B:201:GLY:O	1:B:202:GLU:HB2	2.12	0.48
1:C:175:THR:OG1	1:D:175:THR:HG21	2.13	0.48
1:C:5:LEU:O	1:C:9:ARG:HG2	2.15	0.47
1:A:168:GLU:HG3	1:B:171:VAL:HG11	1.97	0.47

All (84) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:C:21:PHE:O	1:C:22:ASP:HB3	2.15	0.47
1:A:81:THR:O	1:A:84:VAL:HG22	2.15	0.46
1:C:36:LEU:HD22	1:C:151:SER:HB3	1.97	0.46
1:B:192:VAL:HA	1:B:195:ILE:HD12	1.97	0.46
1:B:57:THR:HG23	1:B:57:THR:O	2.15	0.46
1:B:211:ILE:HD12	1:B:214:GLU:OE1	2.16	0.46
1:B:121:LEU:HD21	1:B:131:ILE:HG13	1.97	0.46
1:B:178:GLN:NE2	1:B:257:GLU:OE1	2.49	0.45
1:C:32:MET:HE2	1:C:155:VAL:HG22	1.98	0.45
1:A:192:VAL:HA	1:A:195:ILE:HD12	1.98	0.45
1:C:20:LEU:O	1:C:28:PRO:HB3	2.17	0.45
1:B:96:ILE:HG12	1:B:108:ARG:HG2	1.98	0.45
1:D:184:LEU:HD11	1:D:192:VAL:HG21	1.98	0.45
1:A:191:ALA:HB1	1:A:222:ILE:HD13	1.99	0.45
1:A:191:ALA:O	1:A:195:ILE:HG13	2.18	0.44
1:B:199:LEU:HD11	1:B:204:GLY:N	2.32	0.44
1:A:235:ILE:HA	1:A:248:LYS:O	2.17	0.44
1:D:36:LEU:HD11	1:D:155:VAL:CG2	2.48	0.44
1:C:57:THR:HG23	1:C:57:THR:O	2.17	0.43
1:C:171:VAL:HB	1:D:171:VAL:HG21	2.00	0.43
1:C:153:THR:HG22	1:D:16:GLN:NE2	2.34	0.43
1:C:157:MET:HE2	1:D:123:GLY:HA3	2.01	0.43
1:C:15:LEU:HD21	1:C:35:ILE:HD13	2.00	0.43
1:C:69:ASN:HA	1:C:72:LYS:HE3	2.01	0.43
1:B:192:VAL:CG2	1:B:225:ALA:HB1	2.49	0.42
1:B:179:MET:O	1:B:183:THR:HG23	2.19	0.42
1:D:192:VAL:HA	1:D:195:ILE:HD12	2.01	0.42
1:D:234:ILE:HG22	1:D:234:ILE:O	2.19	0.42
1:D:202:GLU:O	1:D:249:VAL:HG23	2.19	0.42
1:A:121:LEU:CD2	1:A:152:ALA:HB1	2.49	0.42
1:B:236:GLU:O	1:B:247:LEU:HA	2.19	0.42
1:C:81:THR:OG1	1:C:82:GLU:OE1	2.37	0.41
1:A:202:GLU:O	1:A:249:VAL:HG23	2.21	0.41
1:A:211:ILE:O	1:A:215:ILE:HG22	2.21	0.41
1:A:157:MET:HG3	1:B:157:MET:HG3	2.03	0.41
1:B:121:LEU:HD23	1:B:152:ALA:HB1	2.01	0.41
1:D:42:SER:OG	1:D:135:ARG:HD3	2.21	0.41
1:A:26:GLU:O	1:A:27:LEU:HD23	2.21	0.41
1:C:13:GLU:OE1	1:C:17:LYS:HE2	2.21	0.41
1:C:32:MET:HE2	1:C:32:MET:HB3	1.91	0.41
1:C:80:TYR:O	1:C:83:ALA:HB3	2.22	0.40



Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:128:LEU:HD21	1:C:160:LEU:HD13	2.03	0.40
1:D:5:LEU:O	1:D:9:ARG:HG2	2.21	0.40
1:D:27:LEU:HB3	1:D:54:LEU:O	2.22	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	Perce	entiles
1	А	259/262~(99%)	255~(98%)	4 (2%)	0	100	100
1	В	261/262~(100%)	256~(98%)	5 (2%)	0	100	100
1	С	174/262~(66%)	171 (98%)	3 (2%)	0	100	100
1	D	260/262~(99%)	257 (99%)	3 (1%)	0	100	100
All	All	954/1048 (91%)	939~(98%)	15 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	А	221/222 (100%)	216~(98%)	5(2%)	50	62
1	В	223/222 (100%)	217~(97%)	6 (3%)	44	55



Mol	Chain	Analysed	Rotameric	Outliers	Perce	ntiles
1	С	153/222~(69%)	153~(100%)	0	100	100
1	D	222/222 (100%)	219~(99%)	3~(1%)	67	78
All	All	819/888~(92%)	805~(98%)	14 (2%)	60	73

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	\mathbf{Res}	Type
1	А	20	LEU
1	А	34	MET
1	А	143	ASP
1	А	193	HIS
1	А	217	ILE
1	В	143	ASP
1	В	205	ARG
1	В	206	LEU
1	В	210	SER
1	В	219	ARG
1	В	259	GLU
1	D	143	ASP
1	D	193	HIS
1	D	259	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains 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	$\langle RSRZ \rangle$	# RSRZ	5> 2	$OWAB(Å^2)$	Q < 0.9
1	А	261/262~(99%)	1.06	42 (16%) 1	1 1	32, 76, 131, 156	0
1	В	262/262~(100%)	1.60	77 (29%) 0	0	27, 55, 171, 190	0
1	С	178/262~(67%)	0.73	20 (11%) 5	5 4	35, 56, 135, 158	0
1	D	262/262~(100%)	1.05	56 (21%) 0	0	29, 57, 145, 158	0
All	All	963/1048~(91%)	1.14	195 (20%)	1 1	27, 59, 152, 190	0

All (195) RSRZ outliers are listed below:

Mol	Chain	\mathbf{Res}	Type	RSRZ
1	А	108	ARG	13.2
1	В	242	MET	11.4
1	В	221	VAL	10.4
1	В	187	SER	9.5
1	В	215	ILE	9.1
1	В	198	ALA	8.9
1	С	177	VAL	8.8
1	В	258	LEU	8.8
1	В	238	ARG	8.8
1	С	180	ALA	8.4
1	D	206	LEU	7.9
1	А	24	GLN	7.3
1	В	205	ARG	7.0
1	А	211	ILE	6.8
1	В	208	ALA	6.8
1	В	24	GLN	6.8
1	В	252	GLN	6.7
1	А	26	GLU	6.5
1	С	181	ILE	6.5
1	D	178	GLN	6.4
1	В	213	ASP	6.3



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Mol	Chain	Res	Type	RSRZ
1	В	222	ILE	6.3
1	В	246	TYR	6.2
1	D	238	ARG	6.2
1	В	23	VAL	6.2
1	В	186	TYR	6.1
1	В	240	LEU	6.0
1	В	256	LYS	6.0
1	В	237	SER	6.0
1	В	260	LYS	5.8
1	В	196	PHE	5.7
1	В	26	GLU	5.6
1	В	259	GLU	5.6
1	С	179	MET	5.6
1	А	23	VAL	5.6
1	С	174	ALA	5.6
1	В	201	GLY	5.5
1	В	216	GLY	5.5
1	В	219	ARG	5.2
1	В	207	THR	5.2
1	D	247	LEU	5.2
1	В	199	LEU	5.2
1	D	200	ASP	5.2
1	А	109	GLU	5.1
1	В	247	LEU	5.1
1	С	176	ALA	5.1
1	В	245	THR	5.1
1	В	210	SER	5.1
1	В	217	ILE	5.0
1	А	200	ASP	5.0
1	D	258	LEU	4.9
1	С	173	SER	4.9
1	В	200	ASP	4.8
1	А	21	PHE	4.7
1	D	196	PHE	4.7
1	D	201	GLY	4.6
1	В	253	GLN	4.6
1	С	178	GLN	4.6
1	С	171	VAL	4.6
1	D	221	VAL	4.5
1	В	244	GLY	4.5
1	А	246	TYR	4.5
1	В	204	GLY	4.5



Mol	Chain	Res	Type	RSRZ
1	D	242	MET	4.4
1	В	190	LYS	4.4
1	D	199	LEU	4.4
1	D	187	SER	4.3
1	А	-1	GLY	4.3
1	А	210	SER	4.2
1	D	228	LYS	4.2
1	D	204	GLY	4.2
1	D	254	PHE	4.2
1	В	227	ARG	4.1
1	В	214	GLU	4.1
1	В	255	ILE	4.1
1	С	71	PHE	4.0
1	А	178	GLN	4.0
1	С	175	THR	3.9
1	В	202	GLU	3.9
1	A	113	PHE	3.9
1	В	254	PHE	3.8
1	В	249	VAL	3.8
1	В	194	ALA	3.8
1	D	245	THR	3.8
1	D	208	ALA	3.7
1	А	207	THR	3.7
1	А	201	GLY	3.7
1	D	180	ALA	3.6
1	D	186	TYR	3.6
1	В	239	SER	3.6
1	В	232	ALA	3.6
1	В	27	LEU	3.6
1	В	218	THR	3.6
1	D	183	THR	3.6
1	В	189	LEU	3.5
1	В	235	ILE	3.5
1	D	229	LEU	3.4
1	В	231	SER	3.4
1	В	234	ILE	3.4
1	D	214	GLU	3.4
1	D	174	ALA	3.3
1	D	259	GLU	3.3
1	D	253	GLN	3.3
1	D	233	GLY	3.3
1	В	257	GLU	3.3



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Mol	Chain	Res	Type	RSRZ
1	С	109	GLU	3.3
1	В	226	LEU	3.2
1	А	219	ARG	3.2
1	D	255	ILE	3.2
1	А	64	ASN	3.2
1	В	233	GLY	3.2
1	С	172	ARG	3.2
1	D	225	ALA	3.1
1	В	209	SER	3.1
1	D	246	TYR	3.1
1	В	192	VAL	3.1
1	D	24	GLN	3.1
1	D	249	VAL	3.0
1	D	172	ARG	3.0
1	В	206	LEU	3.0
1	А	203	GLU	3.0
1	А	197	GLU	3.0
1	D	250	LEU	3.0
1	D	235	ILE	3.0
1	D	209	SER	2.9
1	С	167	ILE	2.9
1	А	196	PHE	2.9
1	D	220	SER	2.8
1	D	227	ARG	2.8
1	D	190	LYS	2.8
1	С	137	GLU	2.8
1	A	184	LEU	2.8
1	D	231	SER	2.8
1	В	21	PHE	2.8
1	A	110	LEU	2.8
1	D	224	ASN	2.8
1	D	26	GLU	2.8
1	A	195	ILE	2.8
1	В	229	LEU	2.7
1	В	212	ALA	2.7
1	В	230	GLU	2.7
1	В	184	LEU	2.7
1	A	112	PRO	2.7
1	A	199	LEU	2.7
1	A	205	ARG	2.7
1	A	259	GLU	2.7
1	D	260	LYS	2.7



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Mol	Chain	Res	Type	RSRZ
1	А	189	LEU	2.6
1	В	22	ASP	2.6
1	D	202	GLU	2.6
1	D	205	ARG	2.6
1	С	73	GLU	2.6
1	D	176	ALA	2.6
1	А	183	THR	2.6
1	С	110	LEU	2.6
1	D	230	GLU	2.6
1	В	248	LYS	2.5
1	А	217	ILE	2.5
1	D	237	SER	2.5
1	A	232	ALA	2.5
1	С	79	GLY	2.5
1	A	212	ALA	2.5
1	В	197	GLU	2.5
1	А	256	LYS	2.5
1	В	220	SER	2.5
1	В	154	VAL	2.5
1	В	243	LYS	2.5
1	D	215	ILE	2.5
1	D	198	ALA	2.4
1	В	185	SER	2.4
1	В	191	ALA	2.4
1	D	207	THR	2.4
1	А	242	MET	2.4
1	С	105	PHE	2.4
1	А	27	LEU	2.4
1	А	177	VAL	2.3
1	А	220	SER	2.3
1	D	191	ALA	2.3
1	В	193	HIS	2.3
1	В	203	GLU	2.3
1	В	15	LEU	2.2
1	A	249	VAL	2.2
1	В	177	VAL	2.2
1	D	184	LEU	2.2
1	В	-1	GLY	2.2
1	A	247	LEU	2.2
1	A	206	LEU	2.1
1	А	154	VAL	2.1
1	D	203	GLU	2.1



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Mol	Chain	Res	Type	RSRZ
1	D	192	VAL	2.1
1	D	211	ILE	2.1
1	С	22	ASP	2.1
1	А	20	LEU	2.0
1	В	167	ILE	2.0
1	D	212	ALA	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.

