



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:47 PM GMT

PDB ID : 4AIB  
Title : Crystal Structure of Ornithine Decarboxylase from Entamoeba histolytica.  
Authors : Preeti, P.; Kumar, P.; Tomar, S.  
Deposited on : 2012-02-09  
Resolution : 2.87 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  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

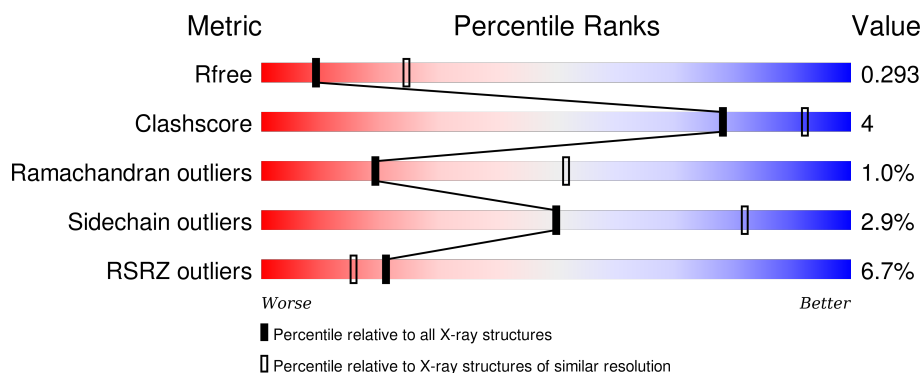
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*





The reported resolution of this entry is 2.87 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))
$R_{free}$	91344	1945 (2.90-2.86)
Clashscore	102246	2202 (2.90-2.86)
Ramachandran outliers	100387	2149 (2.90-2.86)
Sidechain outliers	100360	2152 (2.90-2.86)
RSRZ outliers	91569	1950 (2.90-2.86)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	395	
1	B	395	
1	C	395	
1	D	395	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 10585 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 ORNITHINE DECARBOXYLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	339	Total	C	N	O	S	0	0	0
			2698	1731	446	506	15			
1	B	328	Total	C	N	O	S	0	0	0
			2613	1679	429	489	16			
1	C	323	Total	C	N	O	S	0	0	0
			2575	1657	422	481	15			
1	D	325	Total	C	N	O	S	0	0	0
			2598	1673	425	485	15			

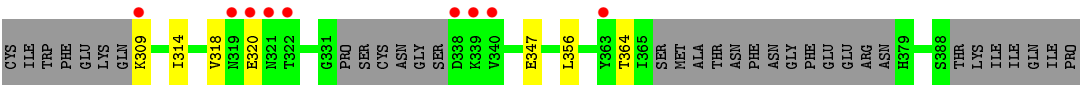
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	38	Total	O	0	0
			38	38		
2	B	24	Total	O	0	0
			24	24		
2	C	24	Total	O	0	0
			24	24		
2	D	15	Total	O	0	0
			15	15		

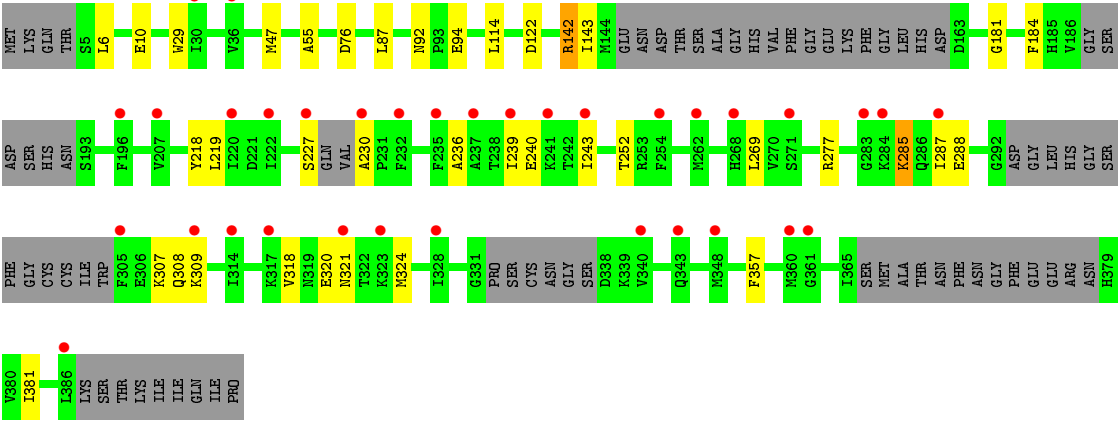


• Molecule 1: ORNITHINE DECARBOXYLASE





● Molecule 1: ORNITHINE DECARBOXYLASE



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	76.67Å 119.28Å 179.29Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	99.50 – 2.87 47.14 – 2.87	Depositor EDS
% Data completeness (in resolution range)	91.8 (99.50-2.87) 91.8 (47.14-2.87)	Depositor EDS
$R_{merge}$	0.15	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.18 (at 2.86Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.253 , 0.299 0.283 , 0.293	Depositor DCC
$R_{free}$ test set	1760 reflections (4.98%)	DCC
Wilson B-factor (Å <sup>2</sup> )	60.8	Xtriage
Anisotropy	0.235	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 41.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	2 of 35410 reflections (0.006%)	Xtriage
$F_o, F_c$ correlation	0.87	EDS
Total number of atoms	10585	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 3.28% 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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.41	1/2756 (0.0%)	0.47	0/3717
1	B	0.41	2/2667 (0.1%)	0.46	0/3596
1	C	0.40	0/2627	0.46	0/3539
1	D	0.40	0/2651	0.46	0/3571
All	All	0.41	3/10701 (0.0%)	0.46	0/14423

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	354	TRP	CD2-CE2	5.07	1.47	1.41
1	A	29	TRP	CD2-CE2	5.04	1.47	1.41
1	B	29	TRP	CD2-CE2	5.01	1.47	1.41

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	2698	0	2678	23	0
1	B	2613	0	2602	17	0
1	C	2575	0	2575	20	0
1	D	2598	0	2593	17	0
2	A	38	0	0	0	0
2	B	24	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	24	0	0	0	0
2	D	15	0	0	0	0
All	All	10585	0	10448	76	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 4.

All (76) 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:C:77:CYS:SG	1:C:96:ILE:HD11	2.10	0.92
1:C:122:ASP:HB3	1:C:142:ARG:HB3	1.72	0.71
1:D:87:LEU:HD13	1:D:114:LEU:HD12	1.74	0.68
1:A:314:ILE:HD13	1:A:356:LEU:HB3	1.76	0.68
1:C:93:PRO:O	1:C:96:ILE:HG22	1.94	0.68
1:C:96:ILE:HG21	1:C:116:ILE:HD12	1.78	0.64
1:C:143:ILE:HG13	1:C:184:PHE:HB3	1.80	0.63
1:C:314:ILE:HD11	1:C:356:LEU:HD22	1.83	0.60
1:B:121:VAL:HG21	1:B:139:ILE:HD11	1.83	0.60
1:C:239:ILE:O	1:C:243:ILE:HG12	2.02	0.58
1:B:16:ILE:HD11	1:B:270:VAL:HG11	1.85	0.58
1:A:60:PRO:HD2	1:A:365:ILE:HD13	1.84	0.58
1:C:51:ARG:HB3	1:C:255:ILE:HG22	1.85	0.57
1:B:143:ILE:HG13	1:B:184:PHE:HB3	1.87	0.57
1:A:329:ILE:HD12	1:A:341:ALA:HB3	1.87	0.56
1:A:280:ILE:HA	1:A:285:LYS:HA	1.87	0.56
1:A:131:ALA:HB2	1:A:177:LEU:HD11	1.89	0.55
1:D:55:ALA:HA	1:D:76:ASP:HB3	1.88	0.55
1:A:55:ALA:HA	1:A:76:ASP:HB3	1.88	0.55
1:C:55:ALA:HA	1:C:76:ASP:HB3	1.88	0.54
1:B:168:VAL:O	1:B:172:ILE:HG12	2.08	0.54
1:B:55:ALA:HA	1:B:76:ASP:HB3	1.91	0.53
1:D:285:LYS:HD3	1:D:287:ILE:HD11	1.92	0.52
1:D:47:MET:HG3	1:D:236:ALA:HB1	1.92	0.51
1:D:239:ILE:HG13	1:D:240:GLU:N	2.24	0.51
1:B:142:ARG:HA	1:B:183:HIS:O	2.10	0.51
1:A:66:LYS:HD3	1:A:89:LEU:HD22	1.93	0.51
1:D:318:VAL:HG22	1:D:320:GLU:H	1.75	0.50
1:C:235:PHE:O	1:C:239:ILE:HG12	2.12	0.49
1:D:29:TRP:HB2	1:D:381:ILE:HG22	1.94	0.49
1:A:47:MET:HG3	1:A:236:ALA:HB1	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:143:ILE:HG13	1:D:184:PHE:HB3	1.95	0.48
1:A:9:LYS:HG3	1:A:314:ILE:HG13	1.94	0.48
1:C:47:MET:HG3	1:C:236:ALA:HB1	1.95	0.48
1:A:190:SER:O	1:A:192:ASN:N	2.47	0.48
1:A:312:GLU:HG3	1:A:314:ILE:CD1	2.43	0.47
1:A:330:TYR:HD1	1:A:338:ASP:O	1.97	0.47
1:C:96:ILE:CG2	1:C:116:ILE:HD12	2.43	0.47
1:D:227:SER:HA	1:D:230:ALA:HB3	1.97	0.47
1:A:280:ILE:HG13	1:A:285:LYS:HB3	1.95	0.47
1:A:105:TYR:HB2	1:B:21:PRO:O	2.14	0.47
1:C:218:TYR:O	1:C:252:THR:HA	2.15	0.47
1:A:142:ARG:HA	1:A:183:HIS:O	2.15	0.46
1:D:92:ASN:ND2	1:D:94:GLU:HB2	2.30	0.46
1:D:6:LEU:O	1:D:10:GLU:HG2	2.16	0.46
1:A:122:ASP:HB3	1:A:142:ARG:HB3	1.98	0.45
1:D:92:ASN:HD21	1:D:94:GLU:HB2	1.81	0.45
1:B:9:LYS:HE2	1:B:314:ILE:HG22	1.97	0.45
1:A:93:PRO:HA	1:A:96:ILE:HD12	1.98	0.45
1:C:77:CYS:HG	1:C:96:ILE:HD11	1.81	0.45
1:B:139:ILE:HG21	1:B:172:ILE:HD12	1.99	0.44
1:B:93:PRO:HA	1:B:96:ILE:HD12	1.99	0.44
1:D:181:GLY:HA3	1:D:219:LEU:O	2.16	0.44
1:B:319:ASN:O	1:B:320:GLU:C	2.56	0.44
1:C:231:PRO:O	1:C:233:GLU:N	2.50	0.44
1:D:122:ASP:HB3	1:D:142:ARG:HB3	2.00	0.44
1:B:233:GLU:HB3	2:B:2017:HOH:O	2.17	0.44
1:D:277:ARG:HB3	1:D:288:GLU:HB2	1.99	0.44
1:C:66:LYS:HB2	1:C:89:LEU:HD22	2.00	0.44
1:C:126:GLU:O	1:C:130:ILE:HG12	2.19	0.43
1:A:142:ARG:HG2	1:A:159:GLY:HA2	2.00	0.43
1:C:121:VAL:HG13	1:C:126:GLU:HB3	2.00	0.43
1:B:66:LYS:HD3	1:B:89:LEU:HD22	2.01	0.42
1:D:269:LEU:HB3	1:D:357:PHE:HB2	2.01	0.42
1:A:296:HIS:HB3	1:A:338:ASP:HB2	2.02	0.42
1:C:318:VAL:HG22	1:C:320:GLU:H	1.85	0.42
1:A:181:GLY:HA2	1:A:217:PRO:HB3	2.02	0.42
1:B:181:GLY:HA2	1:B:217:PRO:HB3	2.01	0.41
1:A:309:LYS:HD3	1:A:310:SER:H	1.85	0.41
1:B:230:ALA:HA	1:B:231:PRO:HD3	1.93	0.41
1:A:181:GLY:HA3	1:A:219:LEU:O	2.20	0.41
1:B:271:SER:HB3	1:B:291:SER:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:331:GLY:HA3	1:B:332:PRO:HD3	1.92	0.40
1:A:291:SER:O	1:A:293:ASP:N	2.54	0.40
1:D:218:TYR:HA	1:D:252:THR:HG22	2.04	0.40
1:C:130:ILE:HG21	1:C:139:ILE:HD11	2.02	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	A	329/395 (83%)	310 (94%)	13 (4%)	6 (2%)	11	35
1	B	314/395 (80%)	295 (94%)	17 (5%)	2 (1%)	30	65
1	C	309/395 (78%)	292 (94%)	14 (4%)	3 (1%)	19	52
1	D	311/395 (79%)	294 (94%)	16 (5%)	1 (0%)	46	78
All	All	1263/1580 (80%)	1191 (94%)	60 (5%)	12 (1%)	19	52

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	191	HIS
1	A	292	GLY
1	C	232	PHE
1	A	232	PHE
1	A	320	GLU
1	A	158	PHE
1	A	190	SER
1	B	320	GLU
1	C	282	ASN
1	B	333	SER
1	D	309	LYS

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Mol	Chain	Res	Type
1	C	283	GLY

### 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	297/345 (86%)	288 (97%)	9 (3%)	48	81
1	B	289/345 (84%)	284 (98%)	5 (2%)	68	90
1	C	284/345 (82%)	271 (95%)	13 (5%)	33	67
1	D	286/345 (83%)	279 (98%)	7 (2%)	57	85
All	All	1156/1380 (84%)	1122 (97%)	34 (3%)	50	82

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	SER
1	A	7	GLU
1	A	61	GLU
1	A	114	LEU
1	A	295	LEU
1	A	317	LYS
1	A	322	THR
1	A	324	MET
1	A	386	LEU
1	B	16	ILE
1	B	98	TYR
1	B	160	LEU
1	B	322	THR
1	B	386	LEU
1	C	5	SER
1	C	51	ARG
1	C	61	GLU
1	C	96	ILE
1	C	98	TYR
1	C	103	LYS

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Mol	Chain	Res	Type
1	C	196	PHE
1	C	200	LEU
1	C	208	THR
1	C	250	GLU
1	C	309	LYS
1	C	347	GLU
1	C	364	THR
1	D	142	ARG
1	D	243	ILE
1	D	285	LYS
1	D	307	LYS
1	D	308	GLN
1	D	321	ASN
1	D	324	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	81	ASN
1	A	117	ASN
1	A	178	ASN
1	B	316	GLN
1	C	81	ASN
1	C	100	GLN
1	D	81	ASN
1	D	178	ASN
1	D	308	GLN
1	D	321	ASN

### 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 ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

There are no ligands in this entry.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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	339/395 (85%)	0.36	8 (2%) 62 58	15, 40, 72, 86	0
1	B	328/395 (83%)	0.70	31 (9%) 10 6	24, 56, 81, 90	0
1	C	323/395 (81%)	0.56	15 (4%) 36 31	27, 51, 78, 87	0
1	D	325/395 (82%)	0.81	34 (10%) 8 5	30, 65, 87, 92	0
All	All	1315/1580 (83%)	0.60	88 (6%) 21 15	15, 52, 83, 92	0

All (88) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	335	ASN	7.2
1	C	338	ASP	5.8
1	B	334	CYS	5.3
1	C	340	VAL	5.2
1	C	319	ASN	5.1
1	B	227	SER	5.0
1	A	158	PHE	4.5
1	D	227	SER	4.4
1	D	323	LYS	4.2
1	D	220	ILE	3.9
1	D	239	ILE	3.8
1	A	230	ALA	3.8
1	B	196	PHE	3.8
1	C	230	ALA	3.7
1	B	363	TYR	3.6
1	D	243	ILE	3.6
1	D	230	ALA	3.6
1	C	321	ASN	3.5
1	C	282	ASN	3.5
1	B	365	ILE	3.3
1	B	332	PRO	3.3

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Mol	Chain	Res	Type	RSRZ
1	D	196	PHE	3.3
1	B	333	SER	3.3
1	D	305	PHE	3.2
1	D	222	ILE	3.2
1	B	43	TRP	3.2
1	D	30	ILE	3.1
1	D	328	ILE	3.1
1	D	237	ALA	3.1
1	D	340	VAL	3.0
1	D	309	LYS	3.0
1	B	226	PHE	2.9
1	C	339	LYS	2.9
1	B	236	ALA	2.8
1	A	227	SER	2.7
1	D	287	ILE	2.7
1	B	284	LYS	2.7
1	B	232	PHE	2.7
1	D	284	LYS	2.7
1	A	157	LYS	2.7
1	B	239	ILE	2.7
1	B	234	GLU	2.7
1	D	254	PHE	2.7
1	D	386	LEU	2.7
1	B	341	ALA	2.7
1	B	243	ILE	2.6
1	B	144	MET	2.6
1	A	362	ALA	2.6
1	D	321	ASN	2.5
1	C	322	THR	2.5
1	C	320	GLU	2.5
1	D	232	PHE	2.5
1	C	227	SER	2.4
1	D	271	SER	2.4
1	C	309	LYS	2.4
1	D	36	VAL	2.4
1	D	207	VAL	2.4
1	D	241	LYS	2.4
1	B	339	LYS	2.3
1	D	283	GLY	2.3
1	B	200	LEU	2.3
1	B	309	LYS	2.3
1	D	235	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	317	LYS	2.3
1	C	186	VAL	2.3
1	C	363	TYR	2.2
1	B	46	ASN	2.2
1	A	159	GLY	2.2
1	C	172	ILE	2.2
1	D	360	MET	2.2
1	B	141	ILE	2.2
1	A	319	ASN	2.2
1	B	213	PHE	2.1
1	B	212	GLN	2.1
1	B	225	GLY	2.1
1	D	348	MET	2.1
1	B	235	PHE	2.1
1	B	195	VAL	2.1
1	D	262	MET	2.1
1	B	201	THR	2.1
1	D	314	ILE	2.1
1	A	120	ILE	2.1
1	D	361	GLY	2.1
1	B	220	ILE	2.1
1	C	286	GLN	2.1
1	D	268	HIS	2.0
1	D	343	GLN	2.0
1	B	386	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 ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

There are no ligands in this entry.



## 6.5 Other polymers [i](#)

There are no such residues in this entry.