



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 9, 2026 – 10:29 PM UTC

PDB ID : 9GTZ / pdb_00009gtz
Title : Xenopus tropicalis Interleukin Enhancer-Binding Factor 3 (ILF3) and Interleukin Enhancer-Binding Factor 2 (ILF2) heterodimer.
Authors : Talbot, A.J.; Mancini, E.J.
Deposited on : 2024-09-18
Resolution : 2.53 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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

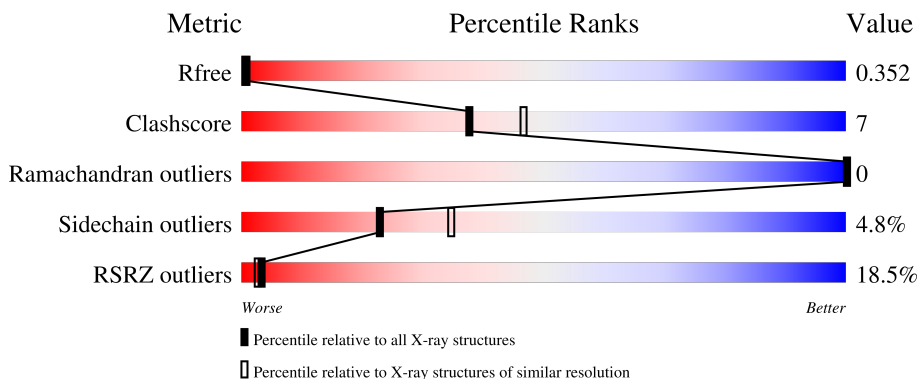
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.53 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}	180053	1091 (2.54-2.54)
Clashscore	190562	1120 (2.54-2.54)
Ramachandran outliers	187476	1106 (2.54-2.54)
Sidechain outliers	187428	1106 (2.54-2.54)
RSRZ outliers	180081	1091 (2.54-2.54)

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 $\leq 5\%$. 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	332	<div> <div>21%</div> <div>82%</div> <div>17%</div> <div>.</div> </div>
2	B	335	<div> <div>14%</div> <div>75%</div> <div>11%</div> <div>13%</div> </div>

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 4786 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 Interleukin enhancer-binding factor 2 homolog.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	332	Total	C	N	O	S	0	6	0
			2460	1557	423	469	11			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	41	SER	THR	conflict	UNP Q6P8G1
A	163	GLY	GLU	conflict	UNP Q6P8G1

- Molecule 2 is a protein called Interleukin enhancer-binding factor 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	291	Total	C	N	O	S	0	6	0
			2183	1374	389	407	13			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	20	SER	VAL	conflict	UNP Q6GL57

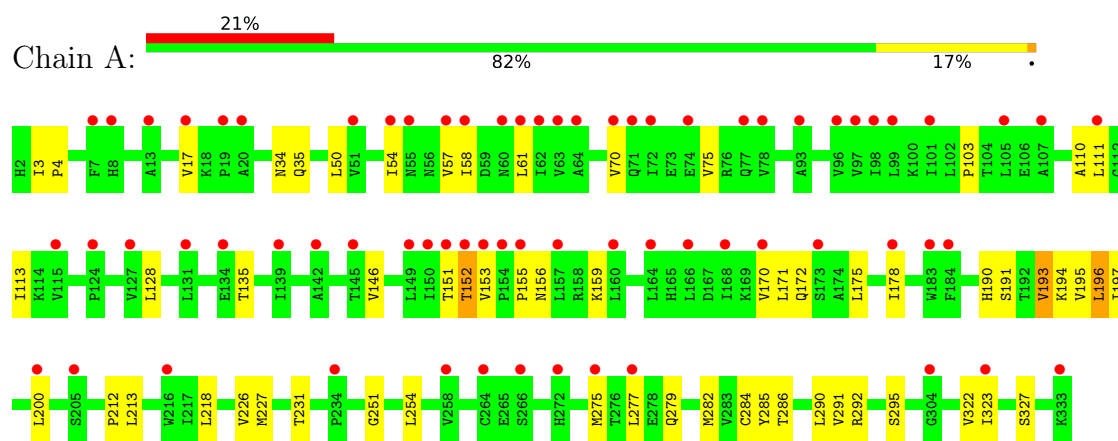
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	74	Total	O	0	0
			74	74		
3	B	69	Total	O	0	0
			69	69		

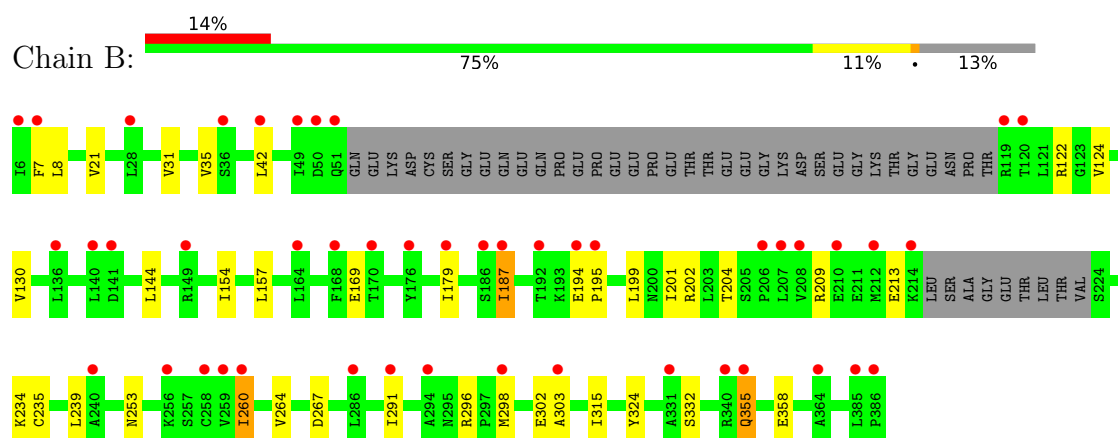
3 Residue-property plots

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: Interleukin enhancer-binding factor 2 homolog



- Molecule 2: Interleukin enhancer-binding factor 3



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	80.97Å 80.97Å 230.36Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	76.82 – 2.53 76.79 – 2.53	Depositor EDS
% Data completeness (in resolution range)	100.0 (76.82-2.53) 99.8 (76.79-2.53)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.24 (at 2.55Å)	Xtriage
Refinement program	PHENIX 1.21.2_5419:	Depositor
R, R_{free}	0.220 , (Not available) 0.288 , 0.352	Depositor DCC
R_{free} test set	1475 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	62.5	Xtriage
Anisotropy	0.014	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 55.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.018 for -h,-k,l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	4786	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.18% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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.

5 Model quality

5.1 Standard geometry

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	0.16	0/2508	0.38	0/3422
2	B	0.16	0/2218	0.39	0/3016
All	All	0.16	0/4726	0.38	0/6438

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

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	2460	0	2387	38	0
2	B	2183	0	2136	31	0
3	A	74	0	0	0	0
3	B	69	0	0	0	0
All	All	4786	0	4523	64	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 7.

All (64) 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:17:VAL:HG22	2:B:324:TYR:HD1	1.10	1.17

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:298:MET:HE3	2:B:302:GLU:HB3	1.39	1.04
1:A:17:VAL:HG22	2:B:324:TYR:CD1	1.92	1.03
1:A:17:VAL:CG2	2:B:324:TYR:HD1	1.90	0.83
2:B:298:MET:HE1	2:B:302:GLU:OE2	1.85	0.76
2:B:298:MET:CE	2:B:302:GLU:HB3	2.18	0.73
2:B:204:THR:HG21	2:B:239:LEU:HG	1.75	0.68
2:B:298:MET:HE1	2:B:302:GLU:CD	2.20	0.67
1:A:251:GLY:HA2	1:A:254:LEU:HD13	1.76	0.65
1:A:58:ILE:HD11	1:A:75:VAL:HG21	1.78	0.65
2:B:260:ILE:O	2:B:264:VAL:HG23	1.98	0.63
1:A:254:LEU:HD11	1:A:284:CYS:HB2	1.82	0.61
1:A:57:VAL:O	1:A:61:LEU:HD12	2.01	0.60
1:A:175:LEU:HA	1:A:178:ILE:HD12	1.84	0.59
1:A:151:THR:HA	1:A:171:LEU:HD22	1.83	0.58
1:A:275:MET:HB3	1:A:279:GLN:HB2	1.83	0.58
1:A:227:MET:HE3	1:A:227:MET:HA	1.86	0.57
2:B:31:VAL:O	2:B:35:VAL:HG23	2.06	0.56
2:B:144:LEU:HG	2:B:199:LEU:HD21	1.89	0.55
2:B:204:THR:HG23	2:B:235[A]:CYS:HB3	1.89	0.55
1:A:212:PRO:HG3	1:A:279:GLN:HB3	1.89	0.55
1:A:190:HIS:HB3	1:A:193:VAL:HG13	1.89	0.55
1:A:322:VAL:HG13	2:B:355:GLN:HG2	1.90	0.53
1:A:17:VAL:HG11	2:B:332:SER:C	2.33	0.53
1:A:191:SER:O	1:A:195:VAL:HG23	2.08	0.53
1:A:285:TYR:HB2	1:A:327:SER:HB2	1.89	0.53
1:A:103[A]:PRO:HD3	1:A:152:THR:HG21	1.91	0.53
2:B:209:ARG:O	2:B:213:GLU:HG3	2.09	0.53
1:A:153:VAL:HB	1:A:155:PRO:HD2	1.91	0.52
2:B:7:PHE:HD2	2:B:302:GLU:HG2	1.74	0.52
2:B:21:VAL:HG21	2:B:267:ASP:HB2	1.93	0.51
2:B:7:PHE:CD2	2:B:302:GLU:HG2	2.47	0.50
2:B:169:GLU:HA	2:B:169:GLU:OE1	2.13	0.49
1:A:50:LEU:HD23	1:A:146:VAL:HG23	1.94	0.49
2:B:202:ARG:HH11	2:B:202:ARG:HG2	1.77	0.48
1:A:58:ILE:HA	1:A:61:LEU:HD12	1.94	0.48
1:A:156:ASN:HA	1:A:159:LYS:HD2	1.95	0.48
1:A:34:ASN:CG	1:A:195:VAL:HG13	2.39	0.47
2:B:298:MET:CE	2:B:302:GLU:CD	2.86	0.47
1:A:193:VAL:HG12	1:A:226:VAL:HG11	1.97	0.47
1:A:282:MET:HA	1:A:285:TYR:CE2	2.51	0.46
2:B:194:GLU:HB3	2:B:195:PRO:HD3	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:213:LEU:HB3	1:A:218:LEU:HD21	1.98	0.45
2:B:202:ARG:HG2	2:B:202:ARG:NH1	2.32	0.45
1:A:3:ILE:HD12	1:A:4:PRO:HD2	1.99	0.45
2:B:298:MET:HE3	2:B:302:GLU:CB	2.28	0.45
1:A:54:ILE:O	1:A:58:ILE:HG23	2.17	0.45
1:A:282:MET:HA	1:A:285:TYR:CZ	2.52	0.45
1:A:58:ILE:HA	1:A:61:LEU:CD1	2.48	0.44
1:A:135:THR:HA	1:A:170:VAL:HG21	2.00	0.44
2:B:42:LEU:HD13	2:B:124:VAL:HG21	1.99	0.44
1:A:193:VAL:O	1:A:197:ILE:HG13	2.17	0.43
2:B:298:MET:CE	2:B:302:GLU:OE2	2.62	0.43
1:A:275:MET:HE3	1:A:275:MET:HB2	1.94	0.43
1:A:196:LEU:O	1:A:200:LEU:HG	2.19	0.42
1:A:110:ALA:O	1:A:113:ILE:HG13	2.20	0.42
1:A:292:ARG:O	1:A:295:SER:HB2	2.20	0.42
2:B:355:GLN:HB2	2:B:358:GLU:HB3	2.01	0.42
2:B:234:LYS:H	2:B:234:LYS:HG2	1.70	0.42
1:A:286:THR:O	1:A:290:LEU:HG	2.19	0.41
2:B:187:ILE:HG23	2:B:201:ILE:HB	2.01	0.41
2:B:296:ARG:CZ	2:B:298:MET:SD	3.09	0.41
2:B:291:ILE:HD11	2:B:303:ALA:HB1	2.03	0.41
1:A:190:HIS:O	1:A:194[A]:LYS:HG3	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	330/332 (99%)	324 (98%)	6 (2%)	0	100	100
2	B	283/335 (84%)	279 (99%)	4 (1%)	0	100	100
All	All	613/667 (92%)	603 (98%)	10 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	257/288 (89%)	245 (95%)	12 (5%)	23	36
2	B	226/292 (77%)	215 (95%)	11 (5%)	22	34
All	All	483/580 (83%)	460 (95%)	23 (5%)	23	35

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	GLN
1	A	70	VAL
1	A	111	LEU
1	A	128	LEU
1	A	152	THR
1	A	172	GLN
1	A	193	VAL
1	A	196	LEU
1	A	231	THR
1	A	277	LEU
1	A	291[A]	VAL
1	A	323	ILE
2	B	8	LEU
2	B	122	ARG
2	B	130	VAL
2	B	154	ILE
2	B	157	LEU
2	B	179	ILE
2	B	187	ILE
2	B	253	ASN
2	B	260	ILE
2	B	315	ILE
2	B	355	GLN

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	223	HIS
1	A	280	GLN
2	B	355	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 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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	340:ARG	C	355:GLN	N	4.77

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, 95th 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	A	332/332 (100%)	1.35	69 (20%) 2 2	39, 64, 101, 120	4 (1%)
2	B	291/335 (86%)	1.22	46 (15%) 5 4	40, 61, 91, 118	5 (1%)
All	All	623/667 (93%)	1.29	115 (18%) 3 3	39, 62, 99, 120	9 (1%)

All (115) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	152	THR	6.0
2	B	298	MET	5.8
1	A	20	ALA	5.2
2	B	36	SER	4.9
1	A	60	ASN	4.9
1	A	57	VAL	4.7
2	B	187	ILE	4.7
2	B	51	GLN	4.6
1	A	62	ILE	4.5
1	A	72	ILE	4.4
1	A	323	ILE	4.3
1	A	17	VAL	4.3
1	A	304	GLY	4.0
1	A	70	VAL	3.9
2	B	286	LEU	3.8
1	A	150	ILE	3.8
2	B	194	GLU	3.8
2	B	210	GLU	3.7
1	A	61	LEU	3.7
1	A	101	ILE	3.7
1	A	183	TRP	3.6
1	A	105	LEU	3.6
1	A	71	GLN	3.6
1	A	99	LEU	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	166	LEU	3.5
1	A	134	GLU	3.3
1	A	111	LEU	3.3
2	B	240	ALA	3.3
2	B	355	GLN	3.2
1	A	154	PRO	3.2
1	A	96	VAL	3.2
1	A	264	CYS	3.2
2	B	50	ASP	3.0
2	B	256	LYS	3.0
2	B	212	MET	3.0
2	B	206	PRO	3.0
1	A	63	VAL	2.9
2	B	6	ILE	2.9
2	B	164	LEU	2.9
2	B	179	ILE	2.9
2	B	140	LEU	2.9
1	A	97	VAL	2.9
2	B	259	VAL	2.9
1	A	107	ALA	2.9
1	A	142	ALA	2.9
1	A	275	MET	2.9
1	A	127	VAL	2.9
1	A	184	PHE	2.9
2	B	149	ARG	2.8
1	A	333	LYS	2.8
2	B	192	THR	2.8
1	A	13	ALA	2.8
2	B	294	ALA	2.8
1	A	55	ASN	2.8
2	B	291	ILE	2.7
2	B	214	LYS	2.7
1	A	272	HIS	2.7
1	A	58	ILE	2.7
1	A	7	PHE	2.6
1	A	98	ILE	2.6
1	A	160	LEU	2.6
1	A	168	ILE	2.5
2	B	120	THR	2.5
2	B	386	PRO	2.5
1	A	139	ILE	2.5
2	B	331	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	151	THR	2.5
2	B	195	PRO	2.5
2	B	49	ILE	2.4
2	B	168	PHE	2.4
1	A	64	ALA	2.4
2	B	119	ARG	2.4
2	B	176	TYR	2.4
1	A	258	VAL	2.4
1	A	93	ALA	2.3
1	A	216	TRP	2.3
1	A	277	LEU	2.3
1	A	153	VAL	2.3
1	A	266	SER	2.3
2	B	28	LEU	2.3
2	B	340	ARG	2.3
1	A	77	GLN	2.2
2	B	207	LEU	2.2
1	A	78	VAL	2.2
1	A	234	PRO	2.2
2	B	258	CYS	2.2
1	A	173	SER	2.2
1	A	205	SER	2.2
2	B	141	ASP	2.2
1	A	51	VAL	2.2
1	A	155	PRO	2.2
2	B	136	LEU	2.2
2	B	7	PHE	2.2
2	B	208	VAL	2.2
1	A	157	LEU	2.2
2	B	385	LEU	2.2
2	B	260	ILE	2.2
1	A	74	GLU	2.2
1	A	19	PRO	2.2
2	B	186	SER	2.1
1	A	8	HIS	2.1
1	A	145	THR	2.1
1	A	124	PRO	2.1
1	A	115	VAL	2.1
1	A	170	VAL	2.1
1	A	131	LEU	2.1
1	A	164	LEU	2.1
2	B	42	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	149	LEU	2.1
2	B	170	THR	2.1
2	B	303	ALA	2.0
1	A	200	LEU	2.0
1	A	54	ILE	2.0
2	B	364	ALA	2.0
1	A	178	ILE	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 oligosaccharides 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.