



# Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 10:47 PM GMT

PDB ID : 2WL8  
Title : X-RAY CRYSTAL STRUCTURE OF PEX19P  
Authors : Schueller, N.; Holton, S.J.; Stanley, W.A.; Song, Y.H.; Konarev, P.; Roessle, M.; Erdmann, R.; Schliebs, W.; Wilmanns, M.  
Deposited on : 2009-06-22  
Resolution : 2.05 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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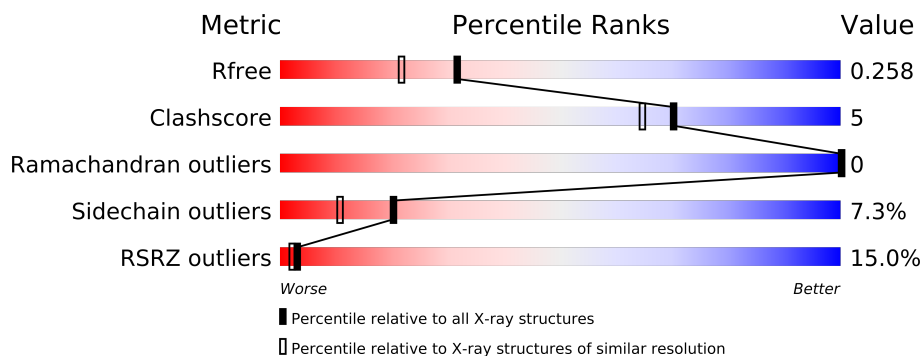
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.05 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))
$R_{free}$	66092	1380 (2.06-2.02)
Clashscore	79885	1577 (2.06-2.02)
Ramachandran outliers	78287	1565 (2.06-2.02)
Sidechain outliers	78261	1565 (2.06-2.02)
RSRZ outliers	66119	1381 (2.06-2.02)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	126	
1	B	126	
1	C	126	
1	D	126	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3715 atoms, of which 0 are hydrogen and 0 are deuterium.

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 PEROXISOMAL BIOGENESIS FACTOR 19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	110	Total	C	N	O	S	0	0	0
			897	570	143	176	8			
1	B	104	Total	C	N	O	S	0	0	0
			850	539	136	167	8			
1	C	109	Total	C	N	O	S	0	0	0
			889	564	142	175	8			
1	D	109	Total	C	N	O	S	0	0	0
			889	564	142	175	8			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	158	GLY	-	EXPRESSION TAG	UNP P40855
A	159	ALA	-	EXPRESSION TAG	UNP P40855
A	160	MET	-	EXPRESSION TAG	UNP P40855
B	158	GLY	-	EXPRESSION TAG	UNP P40855
B	159	ALA	-	EXPRESSION TAG	UNP P40855
B	160	MET	-	EXPRESSION TAG	UNP P40855
C	158	GLY	-	EXPRESSION TAG	UNP P40855
C	159	ALA	-	EXPRESSION TAG	UNP P40855
C	160	MET	-	EXPRESSION TAG	UNP P40855
D	158	GLY	-	EXPRESSION TAG	UNP P40855
D	159	ALA	-	EXPRESSION TAG	UNP P40855
D	160	MET	-	EXPRESSION TAG	UNP P40855

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	50	Total	O	0	0
			50	50		
2	B	75	Total	O	0	0
			75	75		

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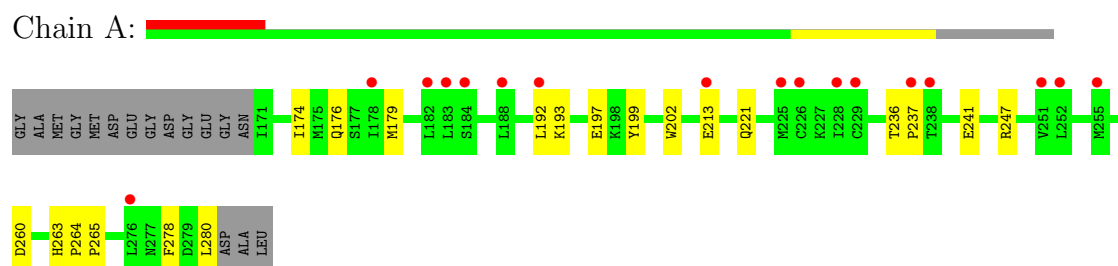
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	C	50	Total	O	0	0
			50	50		
2	D	15	Total	O	0	0
			15	15		

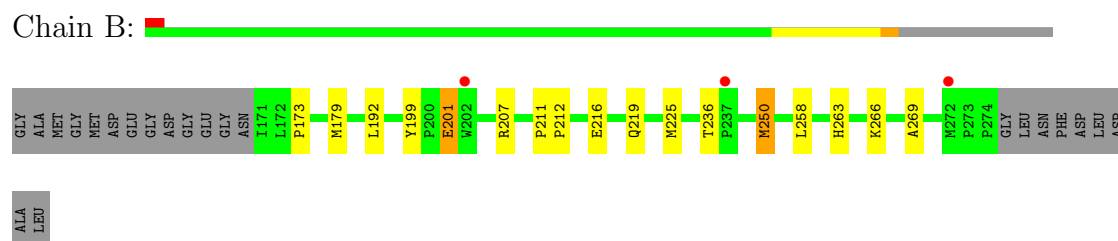
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

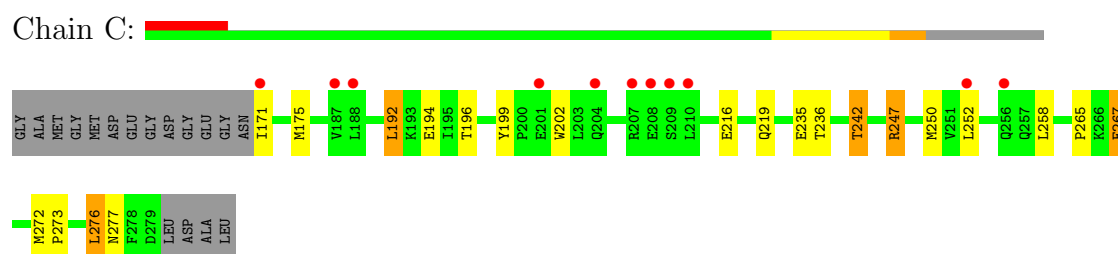
#### • Molecule 1: PEROXISOMAL BIOGENESIS FACTOR 19



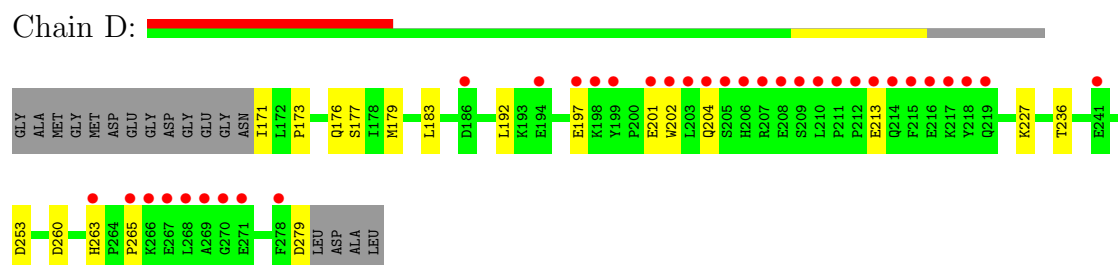
#### • Molecule 1: PEROXISOMAL BIOGENESIS FACTOR 19



#### • Molecule 1: PEROXISOMAL BIOGENESIS FACTOR 19



#### • Molecule 1: PEROXISOMAL BIOGENESIS FACTOR 19



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	67.15Å 91.12Å 122.29Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.45 – 2.05 49.44 – 2.05	Depositor EDS
% Data completeness (in resolution range)	99.1 (49.45-2.05) 99.1 (49.44-2.05)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.30 (at 2.05Å)	Xtriage
Refinement program	REFMAC 5.5.0088	Depositor
R, $R_{free}$	0.199 , 0.239 0.228 , 0.258	Depositor DCC
$R_{free}$ test set	2398 reflections (5.06%)	DCC
Wilson B-factor (Å <sup>2</sup> )	37.3	Xtriage
Anisotropy	0.352	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 45.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 47415 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	3715	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.73% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

## 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	0.66	0/918	0.68	0/1242
1	B	0.81	2/870 (0.2%)	0.73	0/1177
1	C	0.72	0/910	0.85	2/1231 (0.2%)
1	D	0.56	0/910	0.62	0/1231
All	All	0.69	2/3608 (0.1%)	0.73	2/4881 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	173	PRO	N-CD	7.07	1.57	1.47
1	B	199	TYR	CD2-CE2	5.37	1.47	1.39

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	247	ARG	NE-CZ-NH2	-11.79	114.41	120.30
1	C	247	ARG	NE-CZ-NH1	10.37	125.49	120.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	897	0	878	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	850	0	834	9	1
1	C	889	0	867	13	1
1	D	889	0	867	6	0
2	A	50	0	0	0	0
2	B	75	0	0	1	0
2	C	50	0	0	2	0
2	D	15	0	0	0	0
All	All	3715	0	3446	32	1

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 5.

All (32) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:266:LYS:HG2	1:C:194:GLU:HB3	1.65	0.76
1:B:269:ALA:HB3	1:C:194:GLU:HG3	1.75	0.69
1:C:192:LEU:O	1:C:196:THR:HG23	1.94	0.68
1:D:263:HIS:HB3	1:D:279:ASP:HA	1.78	0.66
1:C:242:THR:HG22	2:C:2032:HOH:O	2.00	0.62
1:B:263:HIS:HE1	2:C:2041:HOH:O	1.83	0.60
1:A:193:LYS:O	1:A:197:GLU:HG3	2.02	0.60
1:C:272:MET:H	1:C:277:ASN:HD21	1.51	0.58
1:A:179:MET:HG3	1:C:175:MET:HG2	1.88	0.55
1:C:202:TRP:NE1	1:C:267:GLU:HG2	2.21	0.55
1:C:202:TRP:CZ2	1:C:265:PRO:HB3	2.43	0.53
1:C:202:TRP:HE1	1:C:267:GLU:HG2	1.73	0.53
1:A:221:GLN:HE22	1:A:264:PRO:HA	1.74	0.53
1:B:192:LEU:HD12	1:B:225:MET:HE2	1.91	0.52
1:D:171:ILE:HG13	1:D:173:PRO:HD2	1.92	0.51
1:B:216:GLU:HA	1:B:219:GLN:HE21	1.76	0.50
1:B:192:LEU:CD1	1:B:225:MET:HE2	2.42	0.49
1:C:235:GLU:HG3	1:C:247:ARG:HD3	1.93	0.49
1:B:192:LEU:HD12	1:B:225:MET:CE	2.43	0.48
1:C:216:GLU:HA	1:C:219:GLN:HE21	1.80	0.47
1:A:263:HIS:HD2	1:A:264:PRO:O	1.98	0.46
1:D:202:TRP:CZ2	1:D:265:PRO:HB3	2.51	0.45
1:B:201:GLU:HG3	2:B:2019:HOH:O	2.17	0.45
1:A:260:ASP:OD2	1:D:260:ASP:OD2	2.36	0.44
1:C:273:PRO:O	1:C:276:LEU:HB2	2.18	0.44
1:A:199:TYR:OH	1:A:221:GLN:NE2	2.53	0.42
1:A:263:HIS:HA	1:A:278:PHE:O	2.19	0.42
1:B:211:PRO:HA	1:B:212:PRO:HD3	1.75	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:202:TRP:CZ2	1:A:265:PRO:HB3	2.56	0.41
1:A:236:THR:HB	1:A:237:PRO:HD2	2.02	0.40
1:D:179:MET:CE	1:D:183:LEU:HD11	2.51	0.40
1:C:171:ILE:O	1:D:227:LYS:HE3	2.20	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:250:MET:CE	1:C:250:MET:CE[3_646]	1.98	0.22

## 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	108/126 (86%)	107 (99%)	1 (1%)	0	100	100
1	B	102/126 (81%)	102 (100%)	0	0	100	100
1	C	107/126 (85%)	106 (99%)	1 (1%)	0	100	100
1	D	107/126 (85%)	107 (100%)	0	0	100	100
All	All	424/504 (84%)	422 (100%)	2 (0%)	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	104/113 (92%)	97 (93%)	7 (7%)	23	14

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	99/113 (88%)	93 (94%)	6 (6%)	26	16
1	C	103/113 (91%)	95 (92%)	8 (8%)	18	9
1	D	103/113 (91%)	94 (91%)	9 (9%)	15	7
All	All	409/452 (90%)	379 (93%)	30 (7%)	20	11

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	174	ILE
1	A	176	GLN
1	A	192	LEU
1	A	213	GLU
1	A	241	GLU
1	A	247	ARG
1	A	280	LEU
1	B	179	MET
1	B	201	GLU
1	B	207	ARG
1	B	236	THR
1	B	250	MET
1	B	258	LEU
1	C	192	LEU
1	C	199	TYR
1	C	236	THR
1	C	242	THR
1	C	252	LEU
1	C	258	LEU
1	C	267	GLU
1	C	276	LEU
1	D	176	GLN
1	D	177	SER
1	D	192	LEU
1	D	197	GLU
1	D	201	GLU
1	D	204	GLN
1	D	213	GLU
1	D	236	THR
1	D	253	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	180	GLN
1	A	181	ASN
1	A	204	GLN
1	A	221	GLN
1	A	259	GLN
1	A	263	HIS
1	B	219	GLN
1	B	231	GLN
1	B	263	HIS
1	C	176	GLN
1	C	204	GLN
1	C	219	GLN
1	C	256	GLN
1	C	263	HIS
1	C	277	ASN
1	D	176	GLN
1	D	180	GLN
1	D	221	GLN
1	D	256	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains 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	110/126 (87%)	1.13	17 (15%) 3 2	36, 41, 50, 60	0
1	B	104/126 (82%)	0.77	3 (2%) 49 49	33, 41, 50, 63	0
1	C	109/126 (86%)	1.06	11 (10%) 7 7	33, 41, 51, 58	0
1	D	109/126 (86%)	1.78	34 (31%) 1 0	35, 42, 52, 55	0
All	All	432/504 (85%)	1.19	65 (15%) 3 2	33, 42, 51, 63	0

All (65) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	210	LEU	8.7
1	D	203	LEU	7.1
1	D	213	GLU	6.1
1	D	209	SER	5.9
1	D	208	GLU	5.8
1	D	205	SER	5.7
1	D	267	GLU	5.5
1	D	212	PRO	5.5
1	D	199	TYR	5.3
1	D	207	ARG	5.3
1	D	204	GLN	4.9
1	D	266	LYS	4.8
1	D	198	LYS	4.7
1	D	215	PHE	4.5
1	C	204	GLN	4.3
1	D	202	TRP	4.3
1	D	201	GLU	4.3
1	D	216	GLU	4.3
1	C	208	GLU	3.8
1	D	206	HIS	3.8
1	D	265	PRO	3.8

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Mol	Chain	Res	Type	RSRZ
1	D	269	ALA	3.7
1	C	171	ILE	3.6
1	D	218	TYR	3.4
1	D	214	GLN	3.4
1	D	270	GLY	3.4
1	A	238	THR	3.3
1	D	211	PRO	3.3
1	D	271	GLU	3.2
1	D	268	LEU	3.0
1	A	228	ILE	2.9
1	D	219	GLN	2.8
1	D	217	LYS	2.8
1	C	207	ARG	2.6
1	A	251	VAL	2.6
1	A	226	CYS	2.6
1	A	188	LEU	2.6
1	C	201	GLU	2.6
1	C	210	LEU	2.6
1	D	278	PHE	2.6
1	A	276	LEU	2.5
1	A	255	MET	2.5
1	C	209	SER	2.5
1	B	272	MET	2.4
1	A	213	GLU	2.4
1	A	182	LEU	2.3
1	D	194	GLU	2.3
1	A	229	CYS	2.3
1	A	183	LEU	2.3
1	D	186	ASP	2.3
1	D	263	HIS	2.2
1	D	241	GLU	2.2
1	A	192	LEU	2.2
1	A	178	ILE	2.2
1	C	188	LEU	2.2
1	B	237	PRO	2.2
1	A	225	MET	2.1
1	A	252	LEU	2.1
1	D	197	GLU	2.1
1	C	252	LEU	2.1
1	C	187	VAL	2.1
1	B	202	TRP	2.1
1	A	237	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	184	SER	2.0
1	C	256	GLN	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 ⓘ

There are no such residues in this entry.