



# Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 01:54 am BST

PDB ID : 5KPD  
Title : Mouse pgp 34 linker deleted double EQ mutant  
Authors : Xia, D.; Esser, L.; Zhou, F.  
Deposited on : 2016-07-03  
Resolution : 3.35 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

<https://www.wwpdb.org/validation/2017/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
Xtriage (Phenix)	:	1.13
EDS	:	2.11
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)	:	2.11

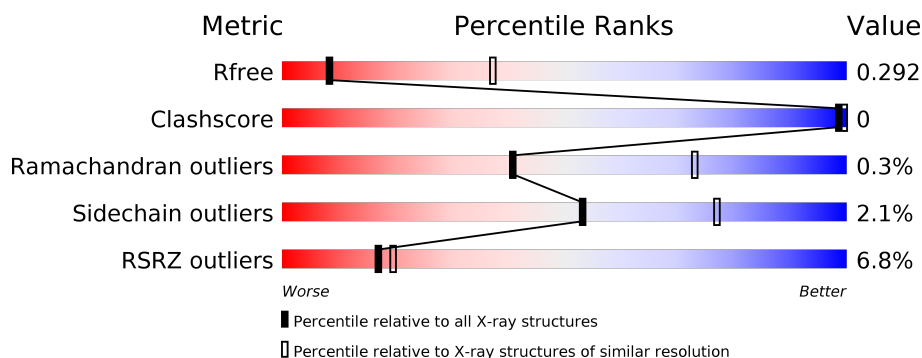
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.35 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))
$R_{free}$	130704	1558 (3.42-3.30)
Clashscore	141614	1627 (3.42-3.30)
Ramachandran outliers	138981	1599 (3.42-3.30)
Sidechain outliers	138945	1598 (3.42-3.30)
RSRZ outliers	127900	1507 (3.42-3.30)

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 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	1248	<div> <div>5%</div> <div> <div></div> <div>91%</div> <div>5%</div> </div> </div>
1	B	1248	<div> <div>8%</div> <div> <div></div> <div>92%</div> <div>5%</div> </div> </div>

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 37084 atoms, of which 18710 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 Multidrug resistance protein 1A.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	1185	Total	C	H	N	O	S	0	0	0
			18546	5907	9357	1559	1685	38			
1	B	1184	Total	C	H	N	O	S	0	0	0
			18538	5905	9353	1558	1684	38			

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	552	GLN	GLU	engineered mutation	UNP P21447
A	?	-	MET	deletion	UNP P21447
A	?	-	SER	deletion	UNP P21447
A	?	-	SER	deletion	UNP P21447
A	?	-	LYS	deletion	UNP P21447
A	?	-	ASP	deletion	UNP P21447
A	?	-	SER	deletion	UNP P21447
A	?	-	GLY	deletion	UNP P21447
A	?	-	SER	deletion	UNP P21447
A	?	-	SER	deletion	UNP P21447
A	?	-	LEU	deletion	UNP P21447
A	?	-	ILE	deletion	UNP P21447
A	?	-	ARG	deletion	UNP P21447
A	?	-	ARG	deletion	UNP P21447
A	?	-	ARG	deletion	UNP P21447
A	?	-	SER	deletion	UNP P21447
A	?	-	THR	deletion	UNP P21447
A	?	-	ARG	deletion	UNP P21447
A	?	-	LYS	deletion	UNP P21447
A	?	-	SER	deletion	UNP P21447
A	?	-	ILE	deletion	UNP P21447
A	?	-	CYS	deletion	UNP P21447
A	?	-	GLY	deletion	UNP P21447
A	?	-	PRO	deletion	UNP P21447
A	?	-	HIS	deletion	UNP P21447

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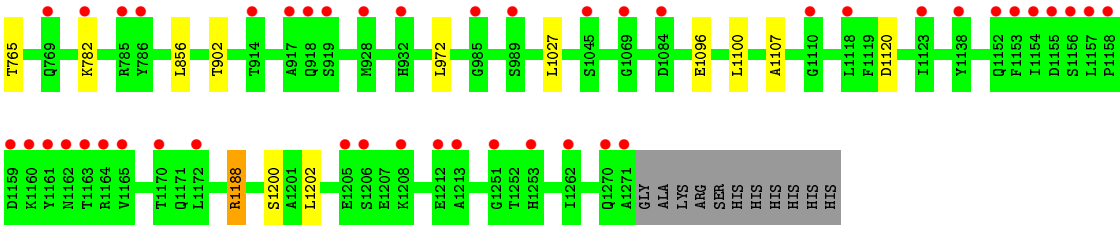
Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	ASP	deletion	UNP P21447
A	?	-	GLN	deletion	UNP P21447
A	?	-	ASP	deletion	UNP P21447
A	?	-	ARG	deletion	UNP P21447
A	?	-	LYS	deletion	UNP P21447
A	?	-	LEU	deletion	UNP P21447
A	?	-	SER	deletion	UNP P21447
A	?	-	THR	deletion	UNP P21447
A	?	-	LYS	deletion	UNP P21447
A	?	-	GLU	deletion	UNP P21447
A	1197	GLN	GLU	engineered mutation	UNP P21447
A	1277	HIS	-	expression tag	UNP P21447
A	1278	HIS	-	expression tag	UNP P21447
A	1279	HIS	-	expression tag	UNP P21447
A	1280	HIS	-	expression tag	UNP P21447
A	1281	HIS	-	expression tag	UNP P21447
A	1282	HIS	-	expression tag	UNP P21447
B	552	GLN	GLU	engineered mutation	UNP P21447
B	?	-	MET	deletion	UNP P21447
B	?	-	SER	deletion	UNP P21447
B	?	-	SER	deletion	UNP P21447
B	?	-	LYS	deletion	UNP P21447
B	?	-	ASP	deletion	UNP P21447
B	?	-	SER	deletion	UNP P21447
B	?	-	GLY	deletion	UNP P21447
B	?	-	SER	deletion	UNP P21447
B	?	-	SER	deletion	UNP P21447
B	?	-	LEU	deletion	UNP P21447
B	?	-	ILE	deletion	UNP P21447
B	?	-	ARG	deletion	UNP P21447
B	?	-	ARG	deletion	UNP P21447
B	?	-	ARG	deletion	UNP P21447
B	?	-	SER	deletion	UNP P21447
B	?	-	THR	deletion	UNP P21447
B	?	-	ARG	deletion	UNP P21447
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B	?	-	SER	deletion	UNP P21447
B	?	-	ILE	deletion	UNP P21447
B	?	-	CYS	deletion	UNP P21447
B	?	-	GLY	deletion	UNP P21447
B	?	-	PRO	deletion	UNP P21447
B	?	-	HIS	deletion	UNP P21447

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Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	ASP	deletion	UNP P21447
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B	?	-	LEU	deletion	UNP P21447
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B	1280	HIS	-	expression tag	UNP P21447
B	1281	HIS	-	expression tag	UNP P21447
B	1282	HIS	-	expression tag	UNP P21447





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	97.95Å 116.59Å 375.56Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	22.42 – 3.35 43.90 – 3.31	Depositor EDS
% Data completeness (in resolution range)	92.9 (22.42-3.35) 91.5 (43.90-3.31)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.18 (at 3.32Å)	Xtriage
Refinement program	PHENIX dev_2443	Depositor
R, $R_{free}$	0.240 , 0.283 0.247 , 0.292	Depositor DCC
$R_{free}$ test set	2408 reflections (4.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	120.8	Xtriage
Anisotropy	0.171	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.26 , 46.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.36$ , $\langle L^2 \rangle = 0.19$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	37084	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	158.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.35% 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, 0.333 respectively for untwinned datasets, and 0.375, 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	0.37	0/9358	0.69	5/12650 (0.0%)
1	B	0.37	0/9354	0.71	3/12645 (0.0%)
All	All	0.37	0/18712	0.70	8/25295 (0.0%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1100	LEU	CA-CB-CG	6.93	131.24	115.30
1	A	1100	LEU	CA-CB-CG	6.45	130.12	115.30
1	A	443	LEU	CB-CG-CD1	5.84	120.93	111.00
1	A	406	LEU	CA-CB-CG	5.37	127.65	115.30
1	A	1218	ARG	NE-CZ-NH1	5.30	122.95	120.30
1	B	406	LEU	CA-CB-CG	5.29	127.46	115.30
1	B	478	THR	OG1-CB-CG2	-5.02	98.46	110.00
1	A	478	THR	OG1-CB-CG2	-5.01	98.48	110.00

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	9189	9357	9374	9	1
1	B	9185	9353	9371	9	1
All	All	18374	18710	18745	17	1

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 0.

All (17) 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:801:ASP:OD2	1:A:1083:TYR:OH	2.21	0.59
1:B:717:ASN:ND2	1:B:765:THR:OG1	2.37	0.54
1:A:278:GLU:OE1	1:A:782:LYS:NZ	2.41	0.52
1:A:478:THR:HG22	1:A:479:THR:H	1.75	0.52
1:B:1107:ALA:O	1:B:1188:ARG:NH2	2.46	0.47
1:A:918:GLN:NE2	1:B:482:GLU:OE2	2.48	0.46
1:B:474:VAL:HG11	1:B:902:THR:HG21	1.97	0.46
1:B:478:THR:HG22	1:B:479:THR:H	1.80	0.46
1:B:737:ASN:OD1	1:B:738:GLY:N	2.49	0.45
1:A:737:ASN:OD1	1:A:738:GLY:N	2.49	0.45
1:B:336:ILE:O	1:B:340:SER:N	2.50	0.44
1:A:852:GLN:N	1:A:852:GLN:OE1	2.51	0.42
1:A:46:ASP:OD1	1:A:138:ARG:NE	2.49	0.42
1:A:417:GLN:HG2	1:A:592:ASP:HB2	2.01	0.42
1:B:278:GLU:OE1	1:B:782:LYS:NZ	2.52	0.42
1:A:507:ASP:OD1	1:A:508:PHE:N	2.53	0.41
1:B:388:LEU:HB2	1:B:413:VAL:HB	2.03	0.41

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	Interatomic distance (Å)	Clash overlap (Å)
1:A:688:VAL:O	1:B:613:ARG:NH1[1_455]	2.19	0.01

## 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	1181/1248 (95%)	1123 (95%)	55 (5%)	3 (0%)	41	73
1	B	1180/1248 (95%)	1120 (95%)	56 (5%)	4 (0%)	41	73
All	All	2361/2496 (95%)	2243 (95%)	111 (5%)	7 (0%)	41	73

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1120	ASP
1	B	1120	ASP
1	A	411	LEU
1	A	556	ALA
1	B	411	LEU
1	B	556	ALA
1	B	691	ALA

### 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	977/1031 (95%)	955 (98%)	22 (2%)	50	75
1	B	977/1031 (95%)	958 (98%)	19 (2%)	57	79
All	All	1954/2062 (95%)	1913 (98%)	41 (2%)	53	77

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	69	LEU
1	A	121	VAL
1	A	299	PHE
1	A	306	TYR
1	A	310	PHE
1	A	314	THR
1	A	415	SER
1	A	439	LEU
1	A	550	LEU

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Mol	Chain	Res	Type
1	A	554	THR
1	A	592	ASP
1	A	602	ILE
1	A	614	GLU
1	A	695	ARG
1	A	697	LEU
1	A	916	TYR
1	A	972	LEU
1	A	1096	GLU
1	A	1155	ASP
1	A	1156	SER
1	A	1200	SER
1	A	1226	ILE
1	B	69	LEU
1	B	121	VAL
1	B	299	PHE
1	B	306	TYR
1	B	310	PHE
1	B	411	LEU
1	B	439	LEU
1	B	550	LEU
1	B	592	ASP
1	B	601	VAL
1	B	614	GLU
1	B	695	ARG
1	B	856	LEU
1	B	972	LEU
1	B	1027	LEU
1	B	1096	GLU
1	B	1188	ARG
1	B	1200	SER
1	B	1202	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	87	ASN
1	A	1020	GLN
1	A	1077	GLN
1	B	717	ASN
1	B	962	GLN
1	B	1020	GLN

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Mol	Chain	Res	Type
1	B	1077	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 carbohydrates 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

### 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	1185/1248 (94%)	0.28	64 (5%)	25 28	71, 136, 214, 294	0
1	B	1184/1248 (94%)	0.48	96 (8%)	12 13	74, 141, 228, 343	0
All	All	2369/2496 (94%)	0.38	160 (6%)	17 20	71, 139, 220, 343	0

All (160) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1161	TYR	8.5
1	A	87	ASN	7.7
1	B	690	PRO	7.1
1	B	1158	PRO	6.6
1	A	1161	TYR	6.4
1	A	1229	ARG	6.2
1	B	1270	GLN	6.1
1	B	28	GLU	5.7
1	A	86	LYS	5.6
1	B	687	ASP	5.6
1	B	161	VAL	5.6
1	B	785	ARG	5.6
1	A	1127	ILE	5.6
1	B	1157	LEU	5.2
1	B	691	ALA	5.1
1	B	273	TYR	5.1
1	A	1228	HIS	5.1
1	B	1162	ASN	5.1
1	A	964	LEU	5.0
1	B	522	GLU	5.0
1	B	277	LEU	4.8
1	B	1159	ASP	4.8
1	B	989	SER	4.7
1	B	1154	ILE	4.5

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Mol	Chain	Res	Type	RSRZ
1	B	1156	SER	4.4
1	B	595	ALA	4.4
1	A	1124	ALA	4.3
1	B	1160	LYS	4.2
1	B	1152	GLN	4.2
1	A	1123	ILE	4.2
1	B	1084	ASP	4.2
1	B	424	ASN	4.1
1	A	1227	ALA	4.0
1	B	421	LEU	3.9
1	B	228	TRP	3.9
1	B	1271	ALA	3.8
1	B	523	ARG	3.8
1	A	1172	LEU	3.7
1	A	1186	LEU	3.7
1	B	415	SER	3.7
1	A	1187	VAL	3.6
1	A	1125	GLU	3.6
1	A	85	SER	3.5
1	B	1165	VAL	3.5
1	A	490	ASP	3.5
1	B	689	PRO	3.5
1	A	204	PHE	3.5
1	A	322	TYR	3.4
1	B	1069	GLY	3.4
1	A	559	THR	3.4
1	B	399	SER	3.3
1	A	526	GLN	3.3
1	B	928	MET	3.3
1	B	423	GLY	3.3
1	B	918	GLN	3.2
1	B	1163	THR	3.2
1	B	985	GLY	3.2
1	B	1170	THR	3.1
1	B	782	LYS	3.1
1	B	1205	GLU	3.1
1	B	618	TYR	3.1
1	B	1153	PHE	3.1
1	A	433	VAL	3.1
1	B	1155	ASP	3.1
1	A	321	GLU	3.0
1	B	597	PHE	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	932	HIS	3.0
1	B	280	ALA	3.0
1	B	622	VAL	3.0
1	B	1172	LEU	3.0
1	A	206	ARG	2.9
1	A	1184	ARG	2.9
1	A	1233	ILE	2.9
1	B	270	LEU	2.9
1	B	786	TYR	2.9
1	B	422	VAL	2.9
1	B	401	LYS	2.8
1	B	416	GLY	2.8
1	B	29	LYS	2.8
1	A	625	GLN	2.8
1	B	603	VAL	2.8
1	B	230	LYS	2.7
1	B	1212	GLU	2.7
1	A	436	MET	2.7
1	A	577	THR	2.7
1	B	917	ALA	2.7
1	B	444	ASP	2.6
1	B	596	GLY	2.6
1	A	578	THR	2.6
1	A	550	LEU	2.6
1	A	579	ILE	2.6
1	B	693	PHE	2.6
1	B	1164	ARG	2.6
1	B	1110	GLY	2.6
1	B	1045	SER	2.6
1	B	617	ILE	2.5
1	A	914	THR	2.5
1	B	1262	ILE	2.5
1	A	882	ASP	2.5
1	B	1206	SER	2.5
1	A	90	ASN	2.4
1	A	312	TYR	2.4
1	A	413	VAL	2.4
1	A	954	ARG	2.4
1	A	572	ALA	2.4
1	B	511	LYS	2.4
1	A	443	LEU	2.4
1	A	959	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	769	GLN	2.4
1	A	597	PHE	2.4
1	B	331	PHE	2.4
1	B	1251	GLY	2.4
1	A	205	THR	2.4
1	A	956	GLY	2.4
1	A	1126	ASN	2.4
1	B	443	LEU	2.3
1	B	1123	ILE	2.3
1	B	41	TYR	2.3
1	A	1180	ILE	2.3
1	B	1118	LEU	2.3
1	A	1257	LEU	2.3
1	A	573	ARG	2.3
1	B	490	ASP	2.3
1	A	1182	ILE	2.2
1	B	594	ILE	2.2
1	B	914	THR	2.2
1	A	549	LEU	2.2
1	A	487	GLY	2.2
1	A	1205	GLU	2.2
1	B	400	ARG	2.2
1	A	1204	THR	2.2
1	B	557	LEU	2.2
1	B	80	SER	2.2
1	A	1177	LYS	2.2
1	A	557	LEU	2.1
1	B	364	ILE	2.1
1	B	919	SER	2.1
1	A	435	LEU	2.1
1	B	688	VAL	2.1
1	A	444	ASP	2.1
1	A	418	THR	2.1
1	A	581	ILE	2.1
1	B	306	TYR	2.1
1	B	489	GLU	2.1
1	A	437	GLN	2.1
1	A	82	GLY	2.1
1	A	548	LEU	2.1
1	B	436	MET	2.1
1	B	611	LEU	2.1
1	A	911	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	402	GLU	2.1
1	B	1138	TYR	2.1
1	A	421	LEU	2.1
1	B	440	TYR	2.1
1	A	793	LEU	2.1
1	B	420	ALA	2.1
1	B	299	PHE	2.0
1	B	1253	HIS	2.0
1	B	1213	ALA	2.0
1	B	1208	LYS	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 carbohydrates 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.