



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 06:41 AM GMT

PDB ID : 4L3B  
Title : X-ray structure of the HRV2 A particle uncoating intermediate  
Authors : Vives-Adrian, L.; Querol-Audi, J.; Garriga, D.; Pous, J.; Verdaguer, N  
Deposited on : 2013-06-05  
Resolution : 6.50 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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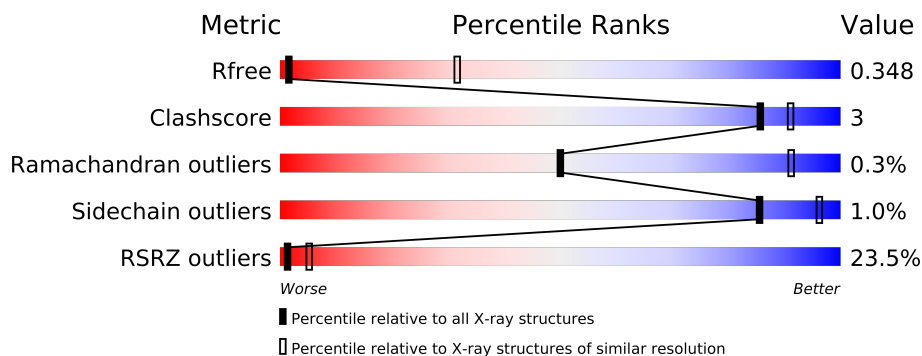
The following versions of software and data (see [references](#)) were used in the production of this report:

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 6.50 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	1097 (9.50-3.50)
Clashscore	79885	1033 (9.00-3.52)
Ramachandran outliers	78287	1291 (9.50-3.50)
Sidechain outliers	78261	1265 (9.50-3.50)
RSRZ outliers	66119	1096 (9.50-3.50)

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	289	
2	B	261	
3	C	237	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5514 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 Protein VP1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	222	Total	C	N	O	S	0	0	0
			1772	1126	310	325	11			

- Molecule 2 is a protein called Protein VP2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	248	Total	C	N	O	S	0	0	0
			1911	1218	328	357	8			

- Molecule 3 is a protein called Protein VP3.

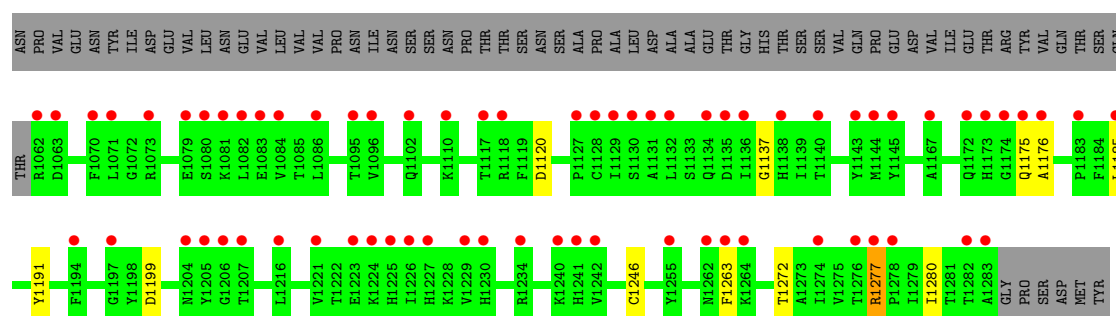
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	237	Total	C	N	O	S	0	0	0
			1831	1169	304	346	12			

### 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.

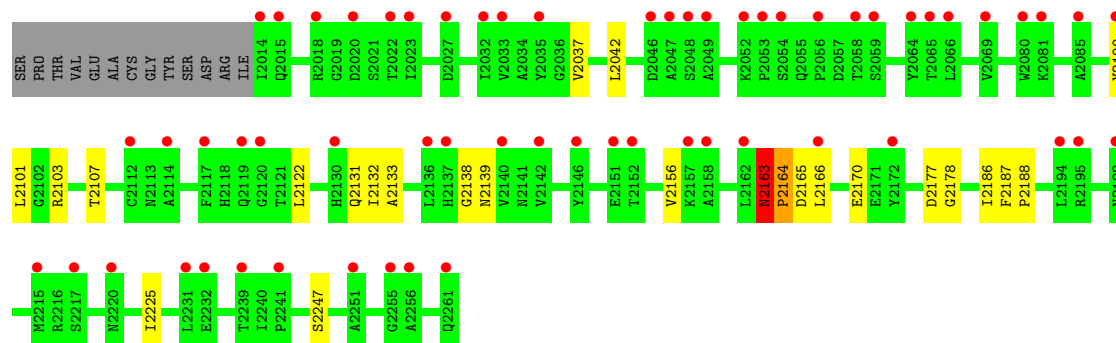
#### • Molecule 1: Protein VP1

Chain A: 



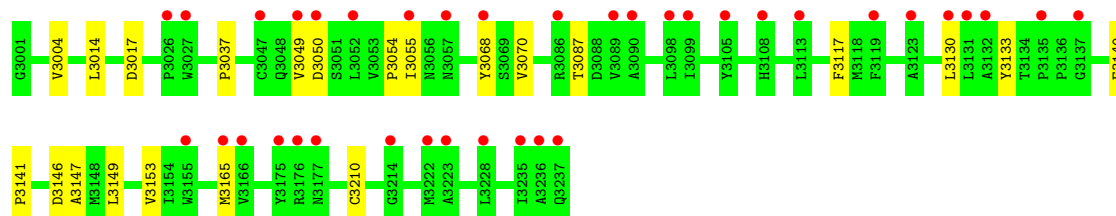
#### • Molecule 2: Protein VP2

Chain B: 



#### • Molecule 3: Protein VP3

Chain C: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	311.93Å 357.83Å 386.67Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	121.39 – 6.50 121.39 – 4.50	Depositor EDS
% Data completeness (in resolution range)	(Not available) (121.39-6.50) 10.6 (121.39-4.50)	Depositor EDS
$R_{merge}$	0.16	Depositor
$R_{sym}$	0.16	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.07 (at 4.47Å)	Xtriage
Refinement program	REFMAC 5.0	Depositor
R, $R_{free}$	0.309 , 0.320 0.348 , 0.348	Depositor DCC
$R_{free}$ test set	813 reflections (5.44%)	DCC
Wilson B-factor (Å <sup>2</sup> )	86.8	Xtriage
Anisotropy	0.280	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 359.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.40$ , $\langle L^2 \rangle = 0.23$	Xtriage
Outliers	0 of 15748 reflections	Xtriage
$F_o, F_c$ correlation	0.61	EDS
Total number of atoms	5514	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	343.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.94% 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	0.28	0/1820	0.49	2/2474 (0.1%)
2	B	0.31	1/1966 (0.1%)	0.50	1/2690 (0.0%)
3	C	0.29	0/1881	0.44	0/2575
All	All	0.29	1/5667 (0.0%)	0.48	3/7739 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2164	PRO	N-CD	5.16	1.55	1.47

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1199	ASP	N-CA-C	6.77	129.28	111.00
1	A	1246	CYS	N-CA-C	6.72	129.16	111.00
2	B	2163	ASN	C-N-CD	5.83	140.65	128.40

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	1772	0	1694	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1911	0	1824	17	0
3	C	1831	0	1804	11	0
All	All	5514	0	5322	29	0

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 3.

All (29) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:2163:ASN:HB3	2:B:2164:PRO:CD	1.97	0.91
2:B:2100:TYR:O	2:B:2101:LEU:HD23	1.84	0.77
2:B:2037:VAL:HG21	3:C:3037:PRO:HB3	1.65	0.76
2:B:2163:ASN:HB3	2:B:2164:PRO:HD2	1.79	0.64
2:B:2165:ASP:CG	2:B:2166:LEU:H	2.05	0.59
2:B:2122:LEU:HD21	2:B:2225:ILE:HG23	1.87	0.57
3:C:3014:LEU:HD23	3:C:3017:ASP:HB3	1.90	0.54
2:B:2165:ASP:O	2:B:2166:LEU:C	2.47	0.53
2:B:2186:ILE:HA	3:C:3049:VAL:HG11	1.90	0.53
2:B:2107:THR:HB	2:B:2247:SER:HB3	1.95	0.47
3:C:3055:ILE:HG21	3:C:3070:VAL:HG22	1.95	0.47
1:A:1175:GLN:HG2	1:A:1176:ALA:H	1.80	0.46
2:B:2131:GLN:H	2:B:2177:ASP:HA	1.81	0.46
1:A:1277:ARG:HG3	1:A:1280:ILE:HG22	1.98	0.45
2:B:2163:ASN:HB3	2:B:2164:PRO:HD3	1.90	0.45
3:C:3153:VAL:HG21	3:C:3165:MET:HG3	1.99	0.44
1:A:1185:LEU:HB2	1:A:1191:TYR:HE2	1.84	0.43
2:B:2042:LEU:HD22	2:B:2103:ARG:HD3	2.01	0.43
2:B:2156:VAL:HG13	2:B:2170:GLU:HB3	2.00	0.43
3:C:3146:ASP:HA	3:C:3149:LEU:HD12	2.00	0.43
3:C:3087:THR:HG21	3:C:3133:TYR:HE1	1.83	0.42
2:B:2187:PHE:O	2:B:2188:PRO:C	2.56	0.42
3:C:3117:PHE:HD1	3:C:3210:CYS:HA	1.85	0.42
1:A:1263:PHE:H	2:B:2133:ALA:HB2	1.84	0.42
3:C:3140:GLU:HA	3:C:3141:PRO:HD3	1.88	0.42
3:C:3054:PRO:HA	3:C:3068:TYR:HA	2.01	0.41
1:A:1263:PHE:HZ	2:B:2178:GLY:HA2	1.84	0.41
2:B:2138:GLY:O	2:B:2139:ASN:C	2.58	0.40
3:C:3130:LEU:HD13	3:C:3147:ALA:HB1	2.02	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	220/289 (76%)	200 (91%)	19 (9%)	1 (0%)	38	88
2	B	246/261 (94%)	204 (83%)	41 (17%)	1 (0%)	43	90
3	C	235/237 (99%)	214 (91%)	21 (9%)	0	100	100
All	All	701/787 (89%)	618 (88%)	81 (12%)	2 (0%)	50	91

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	2163	ASN
1	A	1137	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	187/257 (73%)	184 (98%)	3 (2%)	75	94
2	B	205/226 (91%)	204 (100%)	1 (0%)	94	98
3	C	209/210 (100%)	207 (99%)	2 (1%)	85	96
All	All	601/693 (87%)	595 (99%)	6 (1%)	85	96

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1120	ASP
1	A	1272	THR
1	A	1277	ARG
2	B	2132	ILE

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Mol	Chain	Res	Type
3	C	3004	VAL
3	C	3050	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	2131	GLN
2	B	2218	HIS
3	C	3073	GLN
3	C	3231	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	222/289 (76%)	1.84	69 (31%)	1 4	228, 343, 500, 500	0
2	B	248/261 (95%)	1.41	60 (24%)	1 5	58, 336, 500, 500	7 (2%)
3	C	237/237 (100%)	1.13	37 (15%)	3 9	226, 320, 452, 500	0
All	All	707/787 (89%)	1.45	166 (23%)	1 5	58, 332, 500, 500	7 (0%)

All (166) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1174	GLY	14.8
3	C	3237	GLN	14.1
1	A	1206	GLY	12.1
2	B	2053	PRO	11.1
1	A	1207	THR	9.8
1	A	1131	ALA	9.7
1	A	1225	HIS	9.4
2	B	2215	MET	8.6
1	A	1062	ARG	8.6
3	C	3236	ALA	8.2
1	A	1283	ALA	7.9
2	B	2023	ILE	7.2
1	A	1081	LYS	7.2
2	B	2054	SER	7.1
3	C	3176	ARG	7.1
3	C	3175	TYR	7.1
1	A	1083	GLU	6.9
1	A	1175	GLN	6.5
1	A	1263	PHE	6.5
2	B	2195	ARG	6.4
1	A	1095	THR	6.0
1	A	1129	ILE	6.0
1	A	1176	ALA	5.9

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Mol	Chain	Res	Type	RSRZ
3	C	3235	ILE	5.8
1	A	1132	LEU	5.7
3	C	3165	MET	5.6
2	B	2032	ILE	5.5
1	A	1230	HIS	5.5
3	C	3223	ALA	5.4
2	B	2100	TYR	5.4
1	A	1205	TYR	5.4
1	A	1224	LYS	5.4
1	A	1096	VAL	5.2
1	A	1173	HIS	5.2
2	B	2065	THR	5.0
1	A	1084	VAL	4.9
2	B	2151	GLU	4.7
1	A	1241	HIS	4.6
1	A	1223	GLU	4.5
2	B	2059	SER	4.5
3	C	3137	GLY	4.4
1	A	1130	SER	4.4
2	B	2052	LYS	4.3
1	A	1276	THR	4.2
2	B	2022	THR	4.2
2	B	2015	GLN	4.2
1	A	1226	ILE	4.0
2	B	2172	TYR	3.9
3	C	3055	ILE	3.8
2	B	2251	ALA	3.8
3	C	3099	ILE	3.8
2	B	2047	ALA	3.8
2	B	2048	SER	3.7
1	A	1277	ARG	3.7
2	B	2194	LEU	3.7
1	A	1229	VAL	3.6
3	C	3222	MET	3.6
1	A	1274	ILE	3.6
2	B	2152	THR	3.6
1	A	1082	LEU	3.5
2	B	2241	PRO	3.5
2	B	2137	HIS	3.5
1	A	1143	TYR	3.5
3	C	3098	LEU	3.5
2	B	2231	LEU	3.4

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Mol	Chain	Res	Type	RSRZ
2	B	2014	ILE	3.4
2	B	2136	LEU	3.4
1	A	1278	PRO	3.3
2	B	2256	ALA	3.3
1	A	1262	ASN	3.3
3	C	3086	ARG	3.3
1	A	1135	ASP	3.3
2	B	2198	ASN	3.3
2	B	2146	TYR	3.3
2	B	2232	GLU	3.3
1	A	1134	GLN	3.3
2	B	2018	ARG	3.2
2	B	2112	CYS	3.2
2	B	2058	THR	3.2
1	A	1167	ALA	3.1
1	A	1204	ASN	3.1
2	B	2064	TYR	3.1
2	B	2157	LYS	3.1
2	B	2140	VAL	3.1
2	B	2081	LYS	3.1
3	C	3177	ASN	3.0
2	B	2066	LEU	3.0
2	B	2020	ASP	3.0
3	C	3214	GLY	3.0
2	B	2049	ALA	3.0
1	A	1144	MET	2.9
3	C	3090	ALA	2.9
1	A	1172	GLN	2.9
2	B	2035	TYR	2.9
2	B	2119	GLN	2.9
1	A	1073	ARG	2.9
1	A	1264	LYS	2.8
1	A	1110	LYS	2.8
2	B	2046	ASP	2.7
1	A	1240	LYS	2.7
1	A	1221	VAL	2.7
1	A	1118	ARG	2.7
2	B	2162	LEU	2.7
3	C	3131	LEU	2.7
1	A	1079	GLU	2.7
2	B	2255	GLY	2.6
3	C	3026	PRO	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	1071	LEU	2.6
1	A	1242	VAL	2.6
2	B	2239	THR	2.6
1	A	1234	ARG	2.6
3	C	3068	TYR	2.6
2	B	2085	ALA	2.6
3	C	3135	PRO	2.5
2	B	2033	VAL	2.5
1	A	1255	TYR	2.5
3	C	3089	VAL	2.5
3	C	3123	ALA	2.5
2	B	2217	SER	2.5
1	A	1185	LEU	2.5
3	C	3052	LEU	2.5
2	B	2114	ALA	2.5
1	A	1136	ILE	2.4
2	B	2056	PRO	2.4
3	C	3113	LEU	2.4
3	C	3132	ALA	2.4
3	C	3130	LEU	2.4
1	A	1183	PRO	2.4
2	B	2142	VAL	2.4
1	A	1117	THR	2.4
2	B	2120	GLY	2.4
3	C	3027	TRP	2.4
3	C	3049	VAL	2.4
2	B	2117	PHE	2.4
1	A	1102	GLN	2.3
1	A	1194	PHE	2.3
2	B	2158	ALA	2.3
1	A	1138	HIS	2.3
2	B	2166	LEU	2.3
1	A	1127	PRO	2.3
1	A	1227	HIS	2.3
1	A	1145	TYR	2.2
1	A	1197	GLY	2.2
1	A	1216	LEU	2.2
3	C	3108	HIS	2.2
2	B	2080	TRP	2.2
1	A	1070	PHE	2.2
1	A	1140	THR	2.2
3	C	3228	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	2069	VAL	2.2
2	B	2130	HIS	2.2
1	A	1086	LEU	2.1
3	C	3105	TYR	2.1
1	A	1128	CYS	2.1
1	A	1282	THR	2.1
3	C	3166	VAL	2.1
2	B	2261	GLN	2.1
3	C	3057	ASN	2.1
3	C	3047	CYS	2.1
3	C	3119	PHE	2.1
2	B	2220	ASN	2.1
2	B	2027	ASP	2.1
1	A	1080	SER	2.0
1	A	1063	ASP	2.0
3	C	3050	ASP	2.0
3	C	3155	TRP	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.