



# wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 14, 2020 – 06:45 AM BST

PDB ID : 6PZQ  
Title : Structure of the human respiratory syncytial virus M2-1 protein in complex with a short positive-sense gene-end RNA  
Authors : Gao, Y.; Cao, D.; Liang, B.  
Deposited on : 2019-08-01  
Resolution : 2.70 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.14.4.dev1  
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) : 2.14.4.dev1

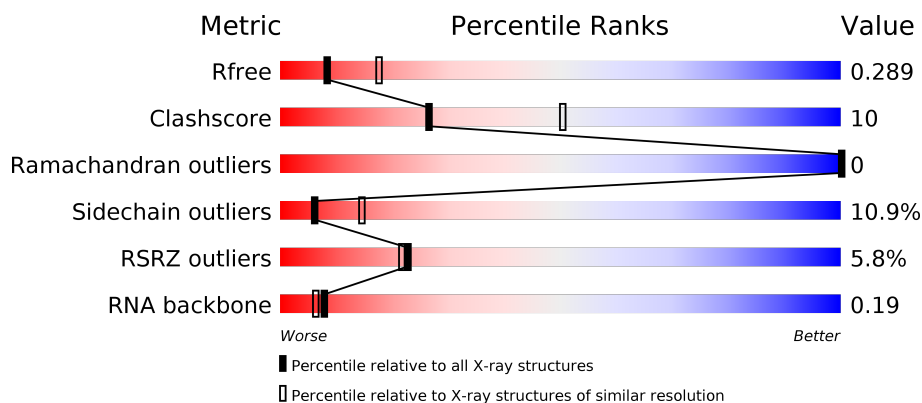
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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.



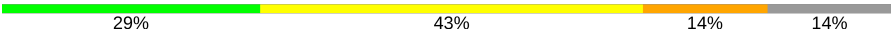

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)
RNA backbone	3102	1159 (3.00-2.40)

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	194	<div> <div>8%</div> <div> <div></div> <div>47%</div> <div>28%</div> <div>6%</div> <div>19%</div> </div> </div>
1	B	194	<div> <div>2%</div> <div> <div></div> <div>55%</div> <div>21%</div> <div>• •</div> <div>20%</div> </div> </div>
1	C	194	<div> <div>3%</div> <div> <div></div> <div>63%</div> <div>13%</div> <div>•</div> <div>22%</div> </div> </div>
1	D	194	<div> <div>6%</div> <div> <div></div> <div>63%</div> <div>15%</div> <div>•</div> <div>20%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
2	I	7	
2	J	7	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	ZN	B	201	-	-	X	-

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 10653 atoms, of which 5324 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 Matrix M2-1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	157	Total	C	H	N	O	S	0	0	0
			2589	802	1314	234	231	8			
1	B	155	Total	C	H	N	O	S	0	0	0
			2558	794	1297	232	228	7			
1	C	152	Total	C	H	N	O	S	0	0	0
			2505	779	1271	226	222	7			
1	D	156	Total	C	H	N	O	S	0	0	0
			2572	798	1303	234	230	7			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	179	LEU	SER	conflict	UNP P04545
B	179	LEU	SER	conflict	UNP P04545
C	179	LEU	SER	conflict	UNP P04545
D	179	LEU	SER	conflict	UNP P04545

- Molecule 2 is a RNA chain called RNA (5'-R(P\*GP\*UP\*UP\*AP\*AP\*U)-3').

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	I	6	Total	C	H	N	O	P	0	0	0
			189	57	64	21	41	6			
2	J	7	Total	C	H	N	O	P	0	0	0
			222	67	75	26	47	7			

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Zn	0	0
			1	1		
3	A	1	Total	Zn	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	1	Total 1	Zn 1	0	0
3	C	1	Total 1	Zn 1	0	0

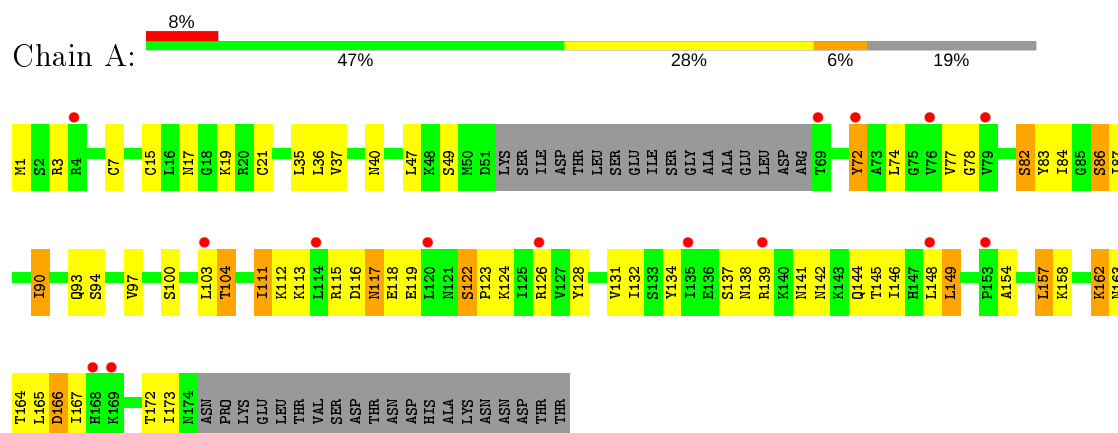
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total 2	O 2	0	0
4	B	8	Total 8	O 8	0	0
4	C	3	Total 3	O 3	0	0
4	I	1	Total 1	O 1	0	0

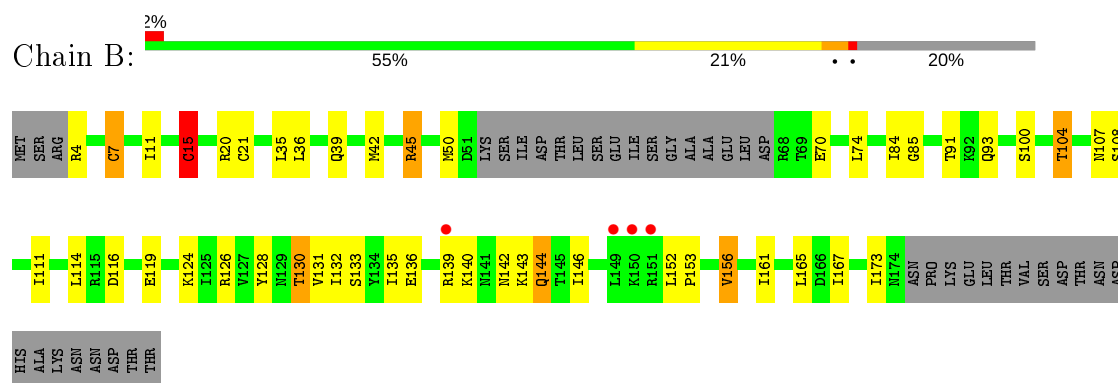
### 3 Residue-property plots [i](#)

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.

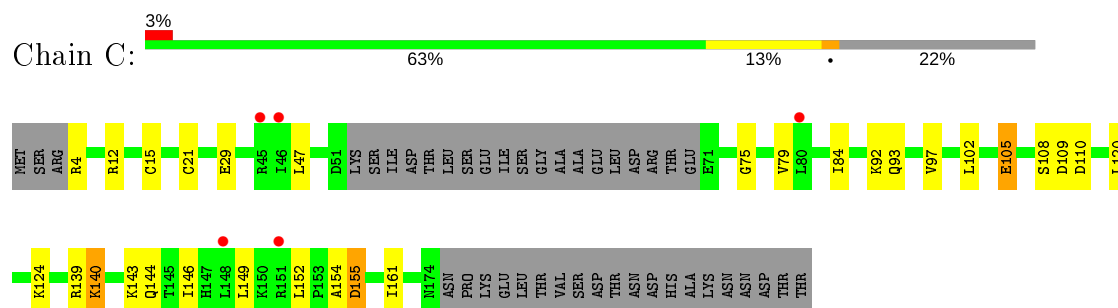
#### • Molecule 1: Matrix M2-1



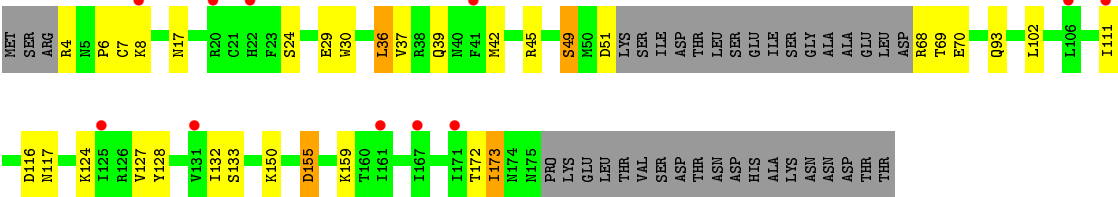
#### • Molecule 1: Matrix M2-1



#### • Molecule 1: Matrix M2-1



#### • Molecule 1: Matrix M2-1



- Molecule 2: RNA (5'-R(P\*GP\*UP\*UP\*AP\*AP\*U)-3')



- Molecule 2: RNA (5'-R(P\*GP\*UP\*UP\*AP\*AP\*U)-3')



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	94.75Å 94.75Å 199.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	63.52 – 2.70 85.60 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.6 (63.52-2.70) 96.5 (85.60-2.70)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.73 (at 2.69Å)	Xtriage
Refinement program	PHENIX 1.11.1 _2575	Depositor
R, $R_{free}$	0.225 , 0.288 0.227 , 0.289	Depositor DCC
$R_{free}$ test set	1282 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	85.8	Xtriage
Anisotropy	0.188	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 65.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	10653	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	104.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.93% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

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	0.73	2/1295 (0.2%)	0.79	0/1741
1	B	0.82	1/1281 (0.1%)	0.87	2/1723 (0.1%)
1	C	0.86	2/1254 (0.2%)	0.81	1/1687 (0.1%)
1	D	0.74	2/1289 (0.2%)	0.77	0/1734
2	I	1.15	1/139 (0.7%)	1.68	3/212 (1.4%)
2	J	0.96	0/164	1.57	0/251
All	All	0.80	8/5422 (0.1%)	0.88	6/7348 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	21	CYS	CB-SG	7.36	1.94	1.82
1	C	15	CYS	CB-SG	-7.07	1.70	1.82
2	I	6	A	N3-C4	6.89	1.39	1.34
1	D	37	VAL	CB-CG1	-6.78	1.38	1.52
1	B	15	CYS	CB-SG	6.03	1.92	1.82

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	15	CYS	CA-CB-SG	9.82	131.68	114.00
1	C	12	ARG	NE-CZ-NH2	-7.67	116.47	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	6	A	N9-C4-C5	-6.43	103.23	105.80
1	B	7	CYS	CA-CB-SG	5.98	124.76	114.00
2	I	3	U	C5'-C4'-O4'	5.68	115.91	109.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	70	GLU	Peptide

## 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	1275	1314	1314	47	0
1	B	1261	1297	1299	33	0
1	C	1234	1271	1271	19	0
1	D	1269	1303	1303	22	0
2	I	125	64	64	0	0
2	J	147	75	75	0	0
3	A	1	0	0	0	0
3	B	1	0	0	2	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	2	0	0	2	0
4	B	8	0	0	1	0
4	C	3	0	0	0	0
4	I	1	0	0	0	0
All	All	5329	5324	5326	109	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 10.

The worst 5 of 109 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:B:7:CYS:HG	3:B:201:ZN:ZN	0.71	0.94
1:B:15:CYS:SG	3:B:201:ZN:ZN	1.64	0.87
1:A:113:LYS:O	1:A:117:ASN:OD1	1.95	0.84
1:B:142:ASN:OD1	1:B:143:LYS:HG3	1.82	0.80
1:B:126:ARG:O	1:B:126:ARG:NH1	2.17	0.76

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	153/194 (79%)	145 (95%)	8 (5%)	0	100	100
1	B	151/194 (78%)	147 (97%)	4 (3%)	0	100	100
1	C	148/194 (76%)	139 (94%)	9 (6%)	0	100	100
1	D	152/194 (78%)	141 (93%)	11 (7%)	0	100	100
All	All	604/776 (78%)	572 (95%)	32 (5%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

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	147/180 (82%)	122 (83%)	25 (17%)	2	5
1	B	145/180 (81%)	127 (88%)	18 (12%)	4	11

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	142/180 (79%)	135 (95%)	7 (5%)	25	52
1	D	146/180 (81%)	133 (91%)	13 (9%)	9	22
All	All	580/720 (81%)	517 (89%)	63 (11%)	6	14

5 of 63 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	45	ARG
1	B	116	ASP
1	D	117	ASN
1	B	50	MET
1	B	93	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	144	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	I	5/7 (71%)	3 (60%)	0
2	J	6/7 (85%)	3 (50%)	0
All	All	11/14 (78%)	6 (54%)	0

5 of 6 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	I	3	U
2	I	4	U
2	I	7	U
2	J	2	G
2	J	5	A

There are no RNA pucker outliers to report.

## 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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	157/194 (80%)	0.71	15 (9%) 8 6	54, 109, 146, 166	0
1	B	155/194 (79%)	0.48	4 (2%) 56 57	51, 87, 125, 136	0
1	C	152/194 (78%)	0.53	5 (3%) 46 46	50, 82, 117, 132	0
1	D	156/194 (80%)	0.62	11 (7%) 16 14	53, 90, 129, 148	0
2	I	6/7 (85%)	-0.21	0 100 100	101, 103, 125, 129	0
2	J	7/7 (100%)	1.37	2 (28%) 0 0	96, 104, 153, 160	0
All	All	633/790 (80%)	0.59	37 (5%) 23 22	50, 92, 136, 166	0

The worst 5 of 37 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	4	ARG	6.1
2	J	2	G	5.7
1	D	171	ILE	4.5
2	J	1	A	4.2
1	A	114	LEU	4.0

### 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 monosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	ZN	B	201	1/1	0.96	0.31	145,145,145,145	0
3	ZN	C	201	1/1	0.98	0.25	85,85,85,85	0
3	ZN	A	201	1/1	0.99	0.25	79,79,79,79	0
3	ZN	D	201	1/1	0.99	0.24	86,86,86,86	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.