



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 13, 2018 – 04:47 pm GMT

PDB ID : 3RMX  
Title : Crystal structure of HCR/D F1240A mutant  
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Deposited on : 2011-04-21  
Resolution : 2.75 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  
Xtriage (Phenix) : 1.13  
EDS : trunk31020  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk31020

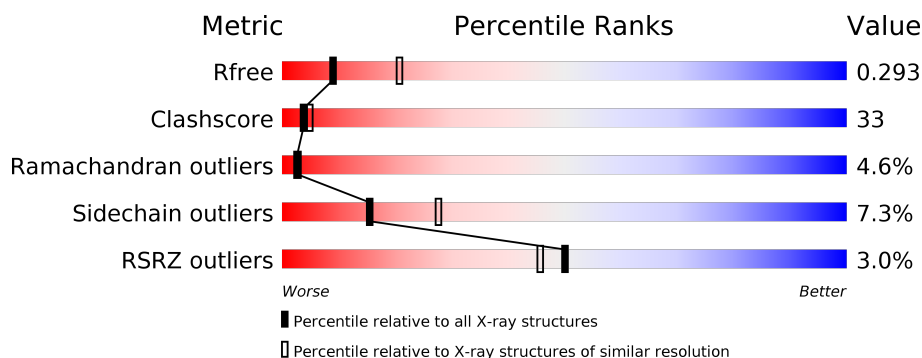
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.75 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))
$R_{free}$	111664	4013 (2.80-2.72)
Clashscore	122126	1029 (2.78-2.74)
Ramachandran outliers	120053	1013 (2.78-2.74)
Sidechain outliers	120020	1013 (2.78-2.74)
RSRZ outliers	108989	3920 (2.80-2.72)

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. 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	415	<div> <div>6%</div> <div>46%</div> <div>44%</div> <div>7%</div> <div>•</div> </div>
1	B	415	<div> <div>42%</div> <div>46%</div> <div>9%</div> <div>•</div> </div>
1	C	415	<div> <div>6%</div> <div>45%</div> <div>44%</div> <div>8%</div> <div>•</div> </div>
1	D	415	<div> <div>3%</div> <div>48%</div> <div>43%</div> <div>6%</div> <div>••</div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 13363 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 Botulinum neurotoxin type D.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	404	Total	C	N	O	S	0	0	0
			3317	2119	548	640	10			
1	B	407	Total	C	N	O	S	0	0	0
			3336	2131	551	644	10			
1	C	403	Total	C	N	O	S	0	0	0
			3304	2111	547	636	10			
1	D	406	Total	C	N	O	S	0	0	0
			3333	2131	550	642	10			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1240	ALA	PHE	ENGINEERED MUTATION	UNP P19321
B	1240	ALA	PHE	ENGINEERED MUTATION	UNP P19321
C	1240	ALA	PHE	ENGINEERED MUTATION	UNP P19321
D	1240	ALA	PHE	ENGINEERED MUTATION	UNP P19321

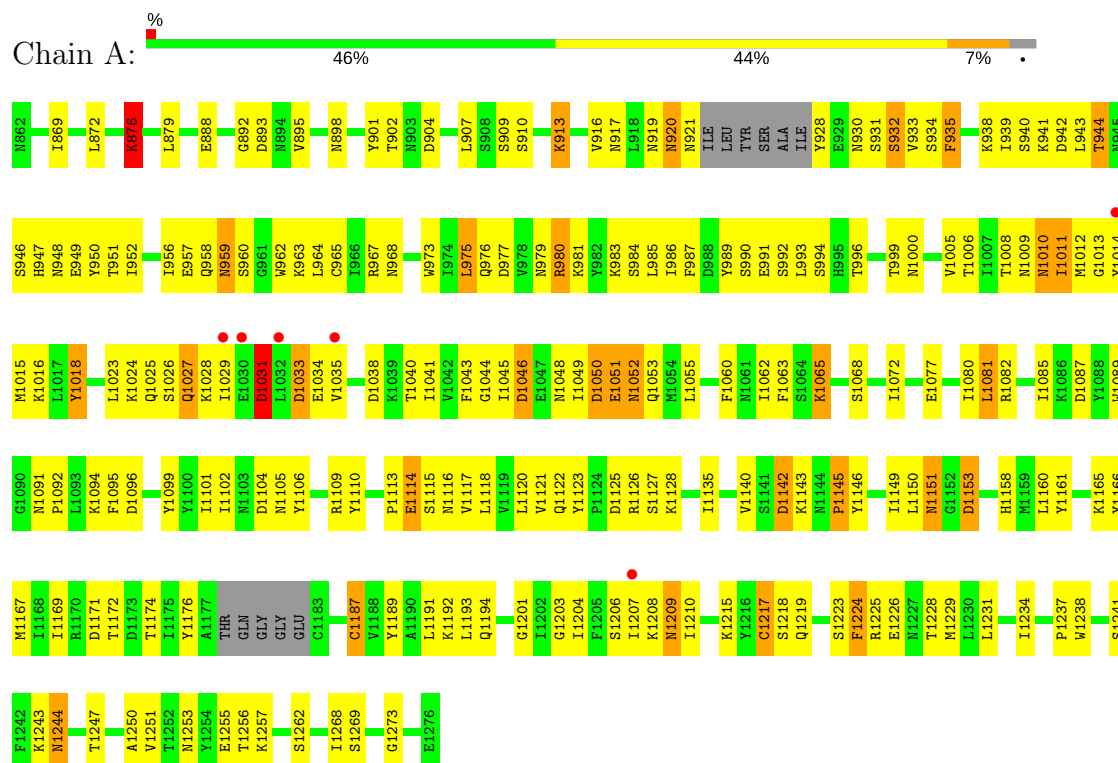
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	19	Total	O	0	0
			19	19		
2	B	18	Total	O	0	0
			18	18		
2	C	17	Total	O	0	0
			17	17		
2	D	19	Total	O	0	0
			19	19		

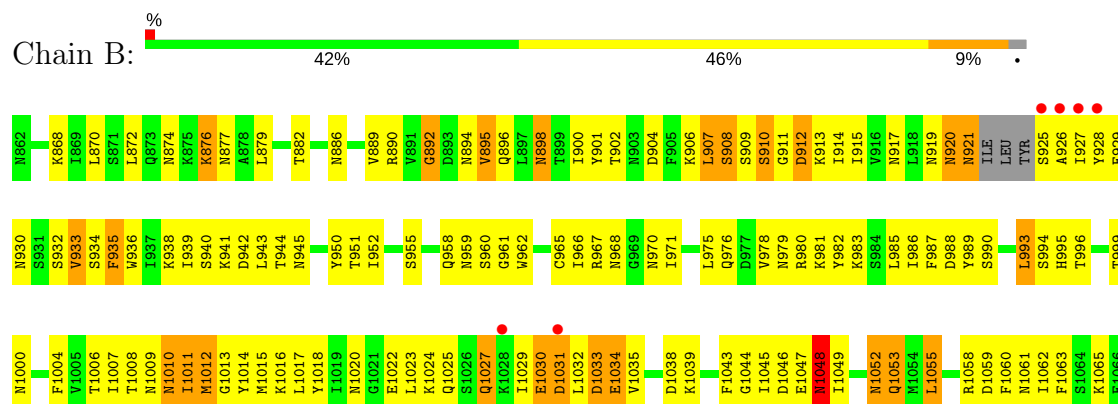
### 3 Residue-property plots

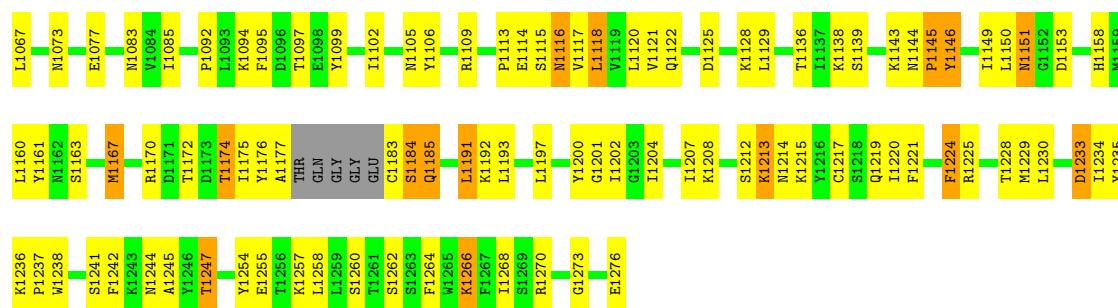
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: Botulinum neurotoxin type D

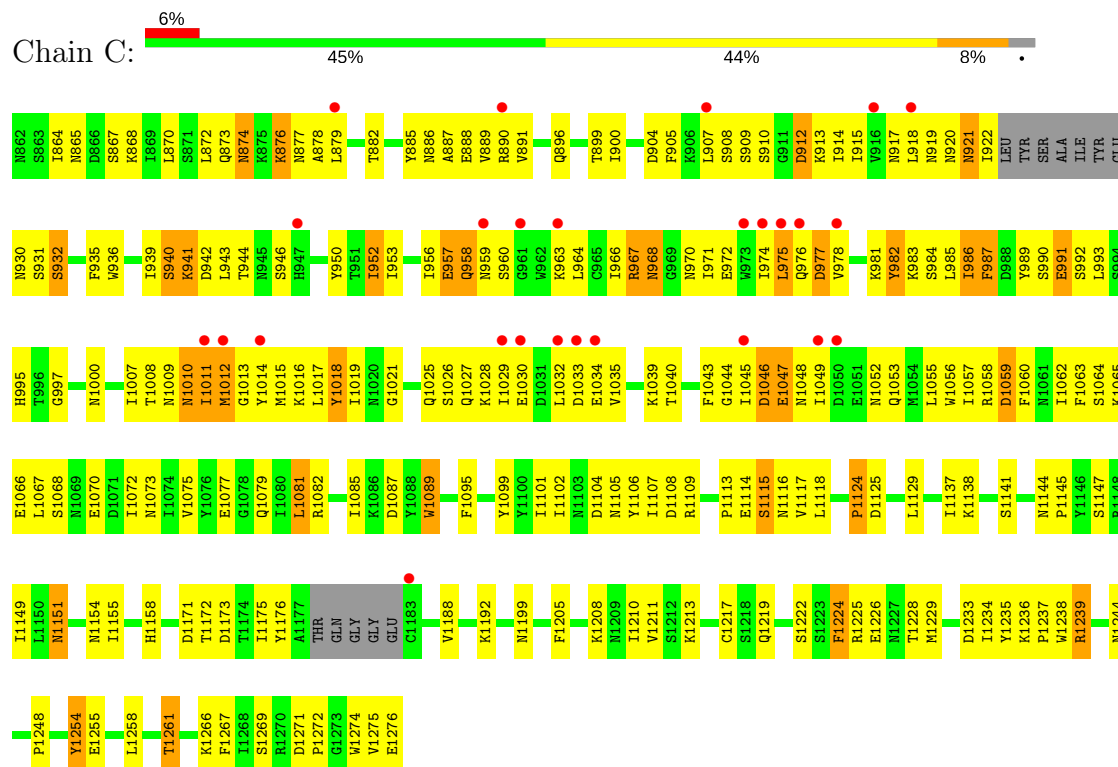


#### • Molecule 1: Botulinum neurotoxin type D

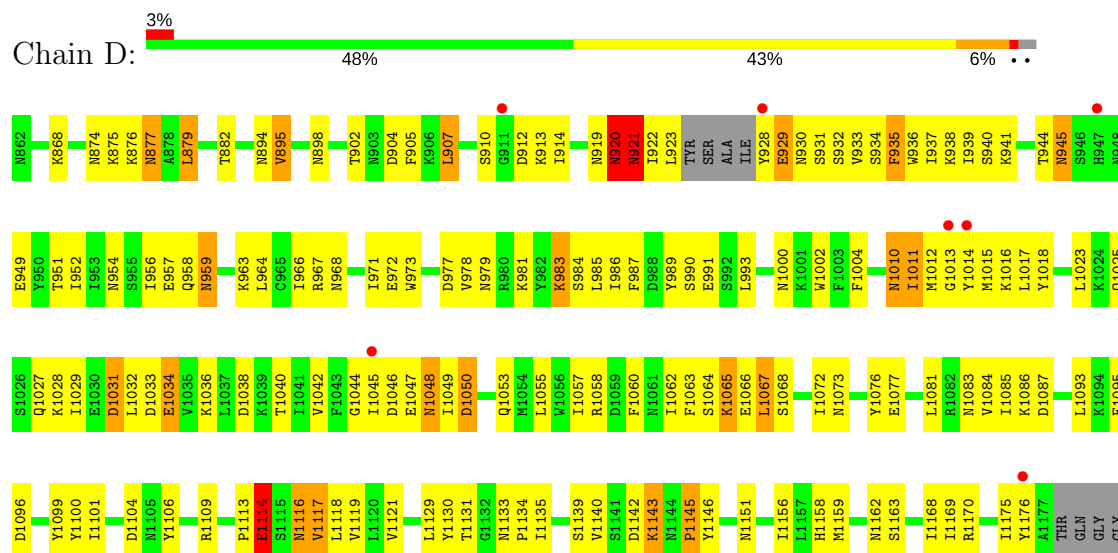




• Molecule 1: Botulinum neurotoxin type D



• Molecule 1: Botulinum neurotoxin type D





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	94.57Å 115.63Å 107.24Å 90.00° 91.91° 90.00°	Depositor
Resolution (Å)	36.61 – 2.75 36.61 – 2.74	Depositor EDS
% Data completeness (in resolution range)	96.3 (36.61-2.75) 95.8 (36.61-2.74)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	6.03 (at 2.72Å)	Xtriage
Refinement program	CNS 1.3	Depositor
R, $R_{free}$	0.239 , 0.293 0.238 , 0.293	Depositor DCC
$R_{free}$ test set	5885 reflections (10.15%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	56.7	Xtriage
Anisotropy	0.174	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 31.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.077 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	13363	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.20% 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	0.43	0/3385	0.66	0/4583
1	B	0.45	0/3404	0.67	0/4609
1	C	0.41	0/3371	0.65	0/4564
1	D	0.43	0/3401	0.65	0/4605
All	All	0.43	0/13561	0.66	0/18361

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 [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	3317	0	3260	196	0
1	B	3336	0	3281	259	0
1	C	3304	0	3256	231	0
1	D	3333	0	3282	188	0
2	A	19	0	0	0	0
2	B	18	0	0	2	0
2	C	17	0	0	1	0
2	D	19	0	0	1	0
All	All	13363	0	13079	865	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 33.



The worst 5 of 865 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:910:SER:HB3	1:B:1048:ASN:HA	1.36	1.08
1:B:1114:GLU:HG3	1:B:1115:SER:H	1.10	1.07
1:B:943:LEU:HD13	1:B:1053:GLN:HE22	1.17	1.05
1:B:927:ILE:HG22	1:B:1029:ILE:HD13	1.37	1.05
1:C:958:GLN:HG2	1:C:959:ASN:H	1.19	1.04

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	398/415 (96%)	328 (82%)	53 (13%)	17 (4%)	3	3
1	B	401/415 (97%)	327 (82%)	57 (14%)	17 (4%)	3	3
1	C	397/415 (96%)	326 (82%)	52 (13%)	19 (5%)	2	2
1	D	400/415 (96%)	340 (85%)	39 (10%)	21 (5%)	2	2
All	All	1596/1660 (96%)	1321 (83%)	201 (13%)	74 (5%)	2	3

5 of 74 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	876	LYS
1	A	920	ASN
1	A	1127	SER
1	A	1142	ASP
1	A	1224	PHE

### 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	378/386 (98%)	349 (92%)	29 (8%)	14	25
1	B	380/386 (98%)	346 (91%)	34 (9%)	11	20
1	C	377/386 (98%)	355 (94%)	22 (6%)	22	40
1	D	380/386 (98%)	354 (93%)	26 (7%)	17	31
All	All	1515/1544 (98%)	1404 (93%)	111 (7%)	15	28

5 of 111 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	1118	LEU
1	B	1266	LYS
1	D	1116	ASN
1	B	1145	PRO
1	B	1174	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 86 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	1151	ASN
1	C	930	ASN
1	D	1116	ASN
1	B	1185	GLN
1	B	1244	ASN

### 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 [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	404/415 (97%)	-0.03	6 (1%) 73 71	28, 60, 94, 106	0
1	B	407/415 (98%)	0.01	6 (1%) 73 71	29, 55, 91, 104	0
1	C	403/415 (97%)	0.27	26 (6%) 19 14	33, 68, 107, 120	0
1	D	406/415 (97%)	0.07	11 (2%) 54 50	31, 60, 96, 105	0
All	All	1620/1660 (97%)	0.08	49 (3%) 50 46	28, 61, 100, 120	0

The worst 5 of 49 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	1183	CYS	7.9
1	C	1034	GLU	7.5
1	C	916	VAL	5.6
1	D	1184	SER	5.5
1	B	927	ILE	5.1

### 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.