



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 09:27 PM GMT

PDB ID : 1OWR  
Title : CRYSTAL STRUCTURE OF HUMAN NFAT1 BOUND MONOMERICALLY TO DNA  
Authors : Stroud, J.C.; Chen, L.  
Deposited on : 2003-03-29  
Resolution : 3.00 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  
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

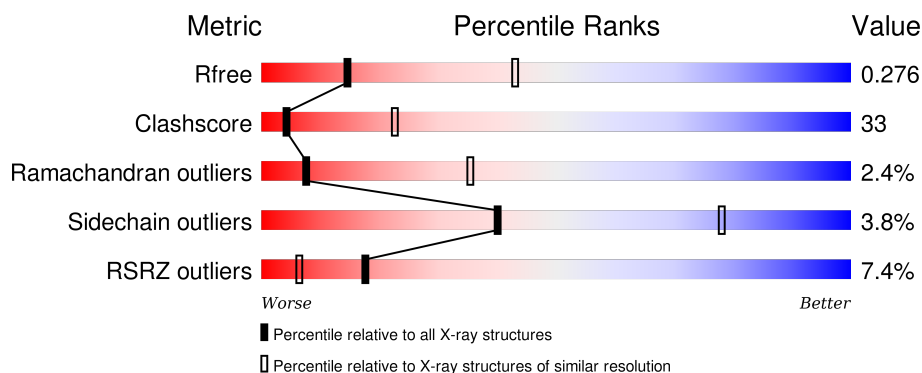
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 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))
$R_{free}$	91344	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)

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	15	<div> <div>7%</div> <div>13%</div> <div>87%</div> </div>
1	C	15	<div> <div>100%</div> </div>
1	E	15	<div> <div>80%</div> <div>20%</div> </div>
1	G	15	<div> <div>7%</div> <div>7%</div> <div>93%</div> </div>
2	B	15	<div> <div>93%</div> <div>7%</div> </div>

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Mol	Chain	Length	Quality of chain
2	D	15	<div><div></div><div>93%</div><div>7%</div></div>
2	F	15	<div><div>7%</div><div>87%</div><div>7%</div></div>
2	H	15	<div><div></div><div>93%</div><div>7%</div></div>
3	M	284	<div><div>12%</div><div>51%</div><div>48%</div><div></div></div>
3	N	284	<div><div>16%</div><div>51%</div><div>44%</div><div>5%</div></div>
3	P	284	<div><div>2%</div><div>56%</div><div>41%</div><div></div></div>
3	Q	284	<div><div>2%</div><div>50%</div><div>49%</div><div></div></div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11436 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 DNA chain called NFAT1 Monomeric Binding Site, Plus Strand.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	15	Total	C	N	O	P	0	0	0
			310	149	61	86	14			
1	C	15	Total	C	N	O	P	0	0	0
			310	149	61	86	14			
1	E	15	Total	C	N	O	P	0	0	0
			310	149	61	86	14			
1	G	15	Total	C	N	O	P	0	0	0
			310	149	61	86	14			

- Molecule 2 is a DNA chain called NFAT1 Monomeric Binding Site, Minus Strand.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	15	Total	C	N	O	P	0	0	0
			299	146	49	90	14			
2	D	15	Total	C	N	O	P	0	0	0
			299	146	49	90	14			
2	F	15	Total	C	N	O	P	0	0	0
			299	146	49	90	14			
2	H	15	Total	C	N	O	P	0	0	0
			299	146	49	90	14			

- Molecule 3 is a protein called Nuclear factor of activated T-cells, cytoplasmic 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	M	284	Total	C	N	O	S	0	0	0
			2250	1414	411	416	9			
3	N	284	Total	C	N	O	S	0	0	0
			2250	1414	411	416	9			
3	P	284	Total	C	N	O	S	0	0	0
			2250	1414	411	416	9			
3	Q	284	Total	C	N	O	S	0	0	0
			2250	1414	411	416	9			

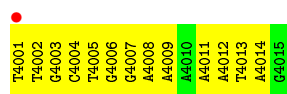
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	395	VAL	-	CLONING ARTIFACT	UNP Q13469
N	395	VAL	-	CLONING ARTIFACT	UNP Q13469
P	395	VAL	-	CLONING ARTIFACT	UNP Q13469
Q	395	VAL	-	CLONING ARTIFACT	UNP Q13469

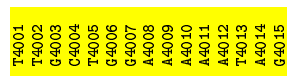
### 3 Residue-property plots

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.

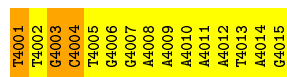
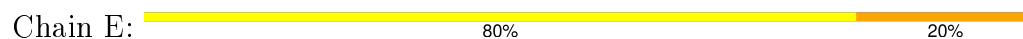
- Molecule 1: NFAT1 Monomeric Binding Site, Plus Strand



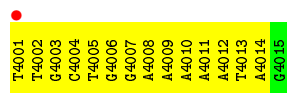
- Molecule 1: NFAT1 Monomeric Binding Site, Plus Strand



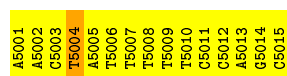
- Molecule 1: NFAT1 Monomeric Binding Site, Plus Strand



- Molecule 1: NFAT1 Monomeric Binding Site, Plus Strand



- Molecule 2: NFAT1 Monomeric Binding Site, Minus Strand



- Molecule 2: NFAT1 Monomeric Binding Site, Minus Strand

Chain D:  93% 7%

A5001  
A5002  
C5003  
T5004  
A5005  
T5006  
T5007  
T5008  
T5009  
T5010  
C5011  
C5012  
A5013  
G5014  
C5015

- Molecule 2: NFAT1 Monomeric Binding Site, Minus Strand

Chain F:  7% 87% 7%

A5001  
A5002  
C5003  
T5004  
A5005  
T5006  
T5007  
T5008  
T5009  
T5010  
C5011  
C5012  
A5013  
G5014  
C5015

- Molecule 2: NFAT1 Monomeric Binding Site, Minus Strand

Chain H:  93% 7%

A5001  
A5002  
C5003  
T5004  
A5005  
T5006  
T5007  
T5008  
T5009  
T5010  
C5011  
C5012  
A5013  
G5014  
C5015

- Molecule 3: Nuclear factor of activated T-cells, cytoplasmic 2

Chain M:  12% 51% 48% .

V895  
P896  
L397  
E398  
W399  
S403  
Q404  
S405  
R411  
I412  
E413  
V414  
Q415  
P416  
K417  
S418  
H419  
R420  
H421  
A422  
H423  
Y424  
E425  
T426  
E427  
G428  
S429  
R430  
G431  
A432  
V433  
K434  
A435  
P436  
T437  
G438  
G439  
H440  
P441  
A442  
V443  
D444  
E450  
N451  
G455  
L456  
Q457  
I458  
F459  
I460  
G461  
T462  
A463  
D464  
E465  
R466  
I467  
L468  
K469  
P470  
H471  
A472  
F473  
Q474  
S475  
L479  
V484  
T485  
T486  
S488  
P489  
V493  
L499  
E500  
Y501  
P502  
L503  
E504  
P505  
M509  
R510  
D514  
C515  
I518  
L519  
K520  
L521  
R522  
N523  
A524  
D525  
V526  
E527  
L528  
R529  
E532  
T533  
D534  
I535  
G536  
N539  
R543  
L544  
V545  
F546  
R547  
E552  
S553  
S554  
G555  
R556  
I557  
L560  
Q561  
N565  
C569  
S570  
Q571  
R572  
S573  
A574  
E575  
E576  
L577  
P578  
V580  
H579  
V580  
E581  
R582  
Q583  
D584  
S587  
C588  
Y591  
Q594  
Q595  
M596  
L597  
L598  
T599  
G600  
Q601  
N602  
F603  
T604  
S605  
E606  
S607  
T612  
E613  
K614  
T615  
T616  
D617  
G618  
Q619  
Q620  
T621  
W622  
T627  
V628  
K629  
K630  
D631  
K632  
S633  
Q634  
P635  
N636  
W637  
L638  
I642  
P643  
E644  
V645  
R646  
N647  
K648  
H649  
I650  
R651  
V656  
V659  
V660  
I661  
N662  
G663  
K664  
R665  
Q671  
T674  
V678

- Molecule 3: Nuclear factor of activated T-cells, cytoplasmic 2

Chain N:  16% 51% 44% 5%

V895  
P896  
L397  
P400  
S403  
Y408  
R411  
I412  
E413  
V414  
Q415  
P416  
K417  
S418  
H419  
R420  
H421  
A422  
H423  
Y424  
E425  
T426  
E427  
R430  
G431  
A432  
V433  
K434  
P436  
H440  
P441  
V442  
Y448  
M449  
E450  
M451  
L456  
Q457  
I458  
F459  
I460  
A463  
I467  
L468  
H471  
A472  
F473  
S475  
L479  
T480  
K482  
T483  
V484  
T485  
T486  
S488  
Y489  
I492  
V493  
L499  
E500  
Y501  
P502  
L503  
E504  
P505  
R510  
A511  
D514  
K520  
L521  
R522  
N523  
A524  
L526  
E527  
T599  
G600  
L601  
N602  
F603  
S605  
V542  
R543  
L544  
V545  
F546  
G618  
R619  
Q620  
L621  
W622  
E623  
T627  
V628  
K630  
D631  
S559  
L560  
Q561  
N565  
P566  
S570  
Q571  
R572  
S573  
A574  
H575  
E576  
L577  
P578  
M579  
V580  
E581  
R582  
Q583  
D584  
T585  
I586  
S587  
C588  
Y591  
G592  
G593  
Q594  
Q595  
L596  
I597  
L598  
T599  
G600  
L601  
N602  
F603  
S605  
R613  
K614  
T615  
T616  
D617  
G618  
Q619  
Q620  
L621  
W622  
E623  
T627  
V628  
K630  
D631





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	100.65Å 94.85Å 112.79Å 90.00° 104.34° 90.00°	Depositor
Resolution (Å)	20.00 – 3.00 20.01 – 2.98	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-3.00) 91.5 (20.01-2.98)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.42 (at 2.98Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.241 , 0.273 0.251 , 0.276	Depositor DCC
$R_{free}$ test set	3420 reflections (9.05%)	DCC
Wilson B-factor (Å <sup>2</sup> )	59.5	Xtriage
Anisotropy	0.697	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 60.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	1 of 39717 reflections (0.003%)	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	11436	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.43% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 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	0.71	0/349	0.89	0/538
1	C	0.63	0/349	0.78	0/538
1	E	0.78	0/349	1.10	3/538 (0.6%)
1	G	0.55	0/349	0.78	0/538
2	B	0.79	0/333	0.99	1/511 (0.2%)
2	D	0.88	1/333 (0.3%)	1.02	1/511 (0.2%)
2	F	0.70	0/333	0.87	0/511
2	H	0.64	0/333	0.81	1/511 (0.2%)
3	M	0.52	0/2300	0.76	0/3115
3	N	0.51	0/2300	0.79	0/3115
3	P	0.49	0/2300	0.74	0/3115
3	Q	0.47	0/2300	0.72	1/3115 (0.0%)
All	All	0.55	1/11928 (0.0%)	0.79	7/16656 (0.0%)

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	E	0	1
2	F	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	5001	DA	N9-C4	-7.20	1.33	1.37

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	4004	DC	O5'-P-OP2	-6.38	99.96	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	5004	DT	OP2-P-O3'	6.15	118.73	105.20
1	E	4004	DC	O4'-C4'-C3'	-5.32	102.37	104.50
2	H	5008	DT	N1-C1'-C2'	5.16	122.40	112.60
2	D	5003	DC	O5'-P-OP2	5.12	116.85	110.70

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	4001	DT	Sidechain
2	F	5002	DA	Sidechain

## 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	310	0	171	33	0
1	C	310	0	171	36	0
1	E	310	0	171	24	0
1	G	310	0	171	36	0
2	B	299	0	173	23	0
2	D	299	0	173	16	0
2	F	299	0	173	23	0
2	H	299	0	173	17	0
3	M	2250	0	2238	142	0
3	N	2250	0	2238	135	0
3	P	2250	0	2238	121	0
3	Q	2250	0	2238	143	0
All	All	11436	0	10328	724	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 724 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:4008:DA:OP1	3:M:665:ARG:HB3	1.37	1.17
1:C:4003:DG:H2''	1:C:4004:DC:H5'	1.20	1.16
3:M:421:ARG:HD2	3:M:571:GLN:HB2	1.27	1.12
1:G:4003:DG:H2''	1:G:4004:DC:H5'	1.21	1.11
1:A:4004:DC:H2''	1:A:4005:DT:H5''	1.16	1.09

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	
3	M	282/284 (99%)	252 (89%)	24 (8%)	6 (2%)	9	40
3	N	282/284 (99%)	251 (89%)	21 (7%)	10 (4%)	4	24
3	P	282/284 (99%)	254 (90%)	21 (7%)	7 (2%)	7	34
3	Q	282/284 (99%)	251 (89%)	27 (10%)	4 (1%)	14	51
All	All	1128/1136 (99%)	1008 (89%)	93 (8%)	27 (2%)	7	35

5 of 27 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	M	635	PRO
3	N	426	THR
3	N	482	LYS
3	P	635	PRO
3	Q	635	PRO

### 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	
3	M	247/254 (97%)	240 (97%)	7 (3%)	51	84
3	N	247/254 (97%)	230 (93%)	17 (7%)	19	56
3	P	247/254 (97%)	240 (97%)	7 (3%)	51	84
3	Q	247/254 (97%)	240 (97%)	7 (3%)	51	84
All	All	988/1016 (97%)	950 (96%)	38 (4%)	40	78

5 of 38 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	N	620	GLN
3	N	653	PRO
3	Q	651	ARG
3	N	627	THR
3	N	667	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 41 such sidechains are listed below:

Mol	Chain	Res	Type
3	N	602	ASN
3	P	507	ASN
3	Q	657	ASN
3	P	415	GLN
3	P	446	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules 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 [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	15/15 (100%)	-0.29	1 (6%) 21 7	34, 44, 84, 95	0
1	C	15/15 (100%)	-0.45	0 100 100	33, 42, 77, 87	0
1	E	15/15 (100%)	-0.09	0 100 100	47, 57, 103, 112	0
1	G	15/15 (100%)	0.12	1 (6%) 21 7	44, 55, 96, 103	0
2	B	15/15 (100%)	-0.19	0 100 100	18, 48, 79, 80	0
2	D	15/15 (100%)	-0.37	0 100 100	27, 45, 62, 63	0
2	F	15/15 (100%)	-0.16	0 100 100	35, 67, 101, 117	0
2	H	15/15 (100%)	-0.14	0 100 100	38, 62, 83, 96	0
3	M	284/284 (100%)	0.38	34 (11%) 6 2	16, 65, 120, 142	0
3	N	284/284 (100%)	0.56	46 (16%) 3 1	17, 76, 124, 141	0
3	P	284/284 (100%)	-0.17	5 (1%) 71 43	22, 54, 94, 130	0
3	Q	284/284 (100%)	-0.09	6 (2%) 67 36	25, 62, 101, 126	0
All	All	1256/1256 (100%)	0.13	93 (7%) 17 6	16, 62, 114, 142	0

The worst 5 of 93 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	N	576	GLU	6.2
3	M	633	SER	6.2
3	M	664	LYS	6.1
3	M	637	MET	5.5
3	M	665	ARG	5.5

### 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 [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.