



Full wwPDB X-ray Structure Validation Report ⓘ

May 17, 2022 – 12:02 PM EDT

PDB ID : 7RH2
Title : IRF4 Transcription factor mutant -K59R
Authors : Williams, S.J.; Sundararaj, S.; Casarotto, M.G.
Deposited on : 2021-07-16
Resolution : 2.47 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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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	:	2.28.1
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)	:	2.28.1

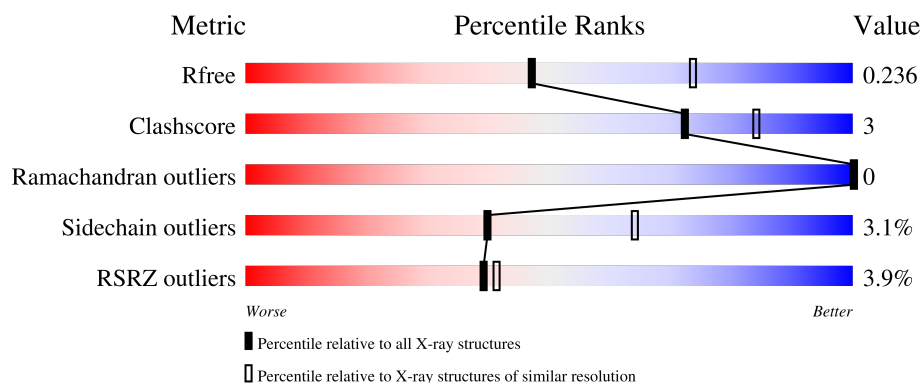
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.47 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	5857 (2.50-2.46)
Clashscore	141614	6594 (2.50-2.46)
Ramachandran outliers	138981	6469 (2.50-2.46)
Sidechain outliers	138945	6471 (2.50-2.46)
RSRZ outliers	127900	5738 (2.50-2.46)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 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	111	<div> <div>0%</div> <div>86%</div> <div>11%</div> <div>..</div> </div>
1	B	111	<div> <div>2%</div> <div>88%</div> <div>9%</div> <div>..</div> </div>
1	G	111	<div> <div>11%</div> <div>88%</div> <div>6%</div> <div>...</div> </div>
1	H	111	<div> <div>4%</div> <div>90%</div> <div>7%</div> <div>..</div> </div>
2	C	19	<div> <div>68%</div> <div>32%</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	D	19	<div><div></div><div>5%</div><div>84%</div><div>16%</div></div>
3	E	19	<div><div></div><div>84%</div><div>16%</div></div>
3	F	19	<div><div></div><div>74%</div><div>16%</div><div>5%</div><div>5%</div></div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9624 atoms, of which 4415 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 ICSAT transcription factor.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	108	Total	C	H	N	O	S	0	0	0
			1807	586	896	161	163	1			
1	B	109	Total	C	H	N	O	S	0	0	0
			1821	590	902	163	165	1			
1	G	109	Total	C	H	N	O	S	0	0	0
			1821	590	902	163	165	1			
1	H	109	Total	C	H	N	O	S	0	0	0
			1821	590	902	163	165	1			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	19	GLY	-	expression tag	UNP Q99419
A	20	SER	-	expression tag	UNP Q99419
A	59	ARG	LYS	engineered mutation	UNP Q99419
B	19	GLY	-	expression tag	UNP Q99419
B	20	SER	-	expression tag	UNP Q99419
B	59	ARG	LYS	engineered mutation	UNP Q99419
G	19	GLY	-	expression tag	UNP Q99419
G	20	SER	-	expression tag	UNP Q99419
G	59	ARG	LYS	engineered mutation	UNP Q99419
H	19	GLY	-	expression tag	UNP Q99419
H	20	SER	-	expression tag	UNP Q99419
H	59	ARG	LYS	engineered mutation	UNP Q99419

- Molecule 2 is a DNA chain called DNA (5'-D(*CP*AP*AP*CP*TP*GP*AP*AP*AP*CP*CP*GP*AP*GP*AP*AP*AP*GP*C)-3').

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	C	19	Total	C	H	N	O	P	0	0	0
			601	185	212	82	104	18			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	D	19	Total	C	H	N	O	P	0	0	0
			603	185	211	82	106	19			

- Molecule 3 is a DNA chain called DNA (5'-D(*GP*CP*TP*TP*TP*CP*TP*CP*GP*GP*TP*TP*TP*CP*AP*GP*TP*TP*G)-3').

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	E	19	Total	C	H	N	O	P	0	0	0
			564	185	182	60	119	18			
3	F	18	Total	C	H	N	O	P	0	0	0
			573	176	208	55	116	18			

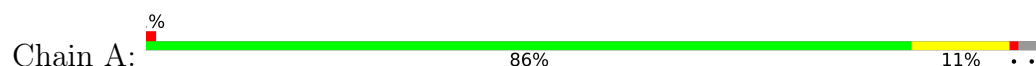
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	3	Total	O	0	0
			3	3		
4	B	4	Total	O	0	0
			4	4		
4	D	1	Total	O	0	0
			1	1		
4	F	1	Total	O	0	0
			1	1		
4	H	4	Total	O	0	0
			4	4		

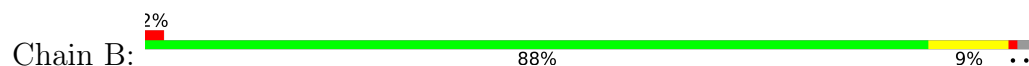
3 Residue-property plots

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.

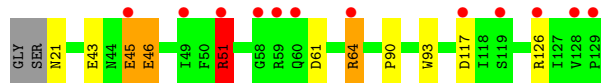
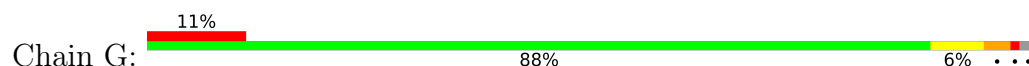
- Molecule 1: ICSAT transcription factor



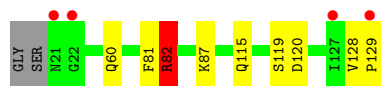
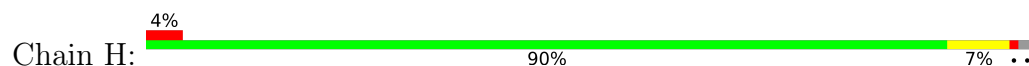
- Molecule 1: ICSAT transcription factor



- Molecule 1: ICSAT transcription factor




- Molecule 1: ICSAT transcription factor



- Molecule 2: DNA (5'-D(*CP*AP*AP*CP*TP*GP*AP*AP*AP*CP*CP*GP*AP*GP*AP*AP*AP*GP*C)-3')




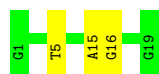
- Molecule 2: DNA (5'-D(*CP*AP*AP*CP*TP*GP*AP*AP*AP*CP*CP*GP*AP*GP*AP*AP*AP*GP*C)-3')

Chain D:  5% 84% 16%



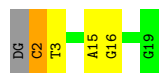
- Molecule 3: DNA (5'-D(*GP*CP*TP*TP*TP*CP*TP*CP*GP*GP*TP*TP*TP*CP*AP*GP*TP*TP*G)-3')

Chain E:  84% 16%



- Molecule 3: DNA (5'-D(*GP*CP*TP*TP*TP*CP*TP*CP*GP*GP*TP*TP*TP*CP*AP*GP*TP*TP*G)-3')

Chain F:  74% 16% 5% 5%



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	114.87Å 114.87Å 154.79Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	46.12 – 2.47 46.12 – 2.47	Depositor EDS
% Data completeness (in resolution range)	99.7 (46.12-2.47) 99.7 (46.12-2.47)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.47 (at 2.48Å)	Xtriage
Refinement program	PHENIX 1.19.1_4122, PHENIX 1.19.1_4122	Depositor
R, R_{free}	0.203 , 0.240 0.201 , 0.236	Depositor DCC
R_{free} test set	2001 reflections (4.70%)	wwPDB-VP
Wilson B-factor (Å ²)	59.8	Xtriage
Anisotropy	0.125	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 33.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.018 for -h,-k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9624	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.66% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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

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	2/937 (0.2%)	0.73	2/1265 (0.2%)
1	B	0.37	0/945	0.73	3/1276 (0.2%)
1	G	0.45	1/945 (0.1%)	0.78	3/1276 (0.2%)
1	H	0.47	2/945 (0.2%)	0.84	4/1276 (0.3%)
2	C	0.80	0/439	0.97	0/675
2	D	0.88	0/442	1.00	0/679
3	E	1.11	0/425	1.28	0/655
3	F	1.14	0/405	1.30	1/623 (0.2%)
All	All	0.70	5/5483 (0.1%)	0.92	13/7725 (0.2%)

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	A	0	2
1	B	0	1
1	G	0	2
1	H	0	1
All	All	0	6

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	82	ARG	CG-CD	15.36	1.90	1.51
1	A	82	ARG	CB-CG	9.20	1.77	1.52
1	H	82	ARG	NE-CZ	-6.42	1.24	1.33
1	G	126	ARG	CB-CG	-5.62	1.37	1.52
1	H	82	ARG	CA-CB	-5.39	1.42	1.53

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	82	ARG	CA-CB-CG	-13.39	83.94	113.40
1	H	82	ARG	NE-CZ-NH1	-12.59	114.01	120.30
1	G	51	ARG	CG-CD-NE	10.59	134.04	111.80
1	B	116	LEU	CA-CB-CG	-10.36	91.46	115.30
1	A	82	ARG	CD-NE-CZ	9.15	136.41	123.60
1	G	51	ARG	NE-CZ-NH2	8.23	124.42	120.30
1	H	82	ARG	NE-CZ-NH2	7.26	123.93	120.30
1	A	82	ARG	CA-CB-CG	7.17	129.17	113.40
1	B	116	LEU	CB-CG-CD2	-6.80	99.43	111.00
1	B	116	LEU	CB-CG-CD1	6.38	121.85	111.00
3	F	2	DC	O4'-C1'-N1	5.53	111.87	108.00
1	H	82	ARG	CB-CA-C	5.23	120.87	110.40
1	G	51	ARG	CD-NE-CZ	-5.14	116.40	123.60

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	126	ARG	Sidechain
1	A	82	ARG	Sidechain
1	B	64	ARG	Sidechain
1	G	51	ARG	Sidechain
1	G	64	ARG	Sidechain
1	H	82	ARG	Sidechain

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	911	896	896	10	0
1	B	919	902	902	5	1
1	G	919	902	902	6	0
1	H	919	902	902	5	1
2	C	389	212	212	3	0
2	D	392	211	211	2	0
3	E	382	182	216	2	0
3	F	365	208	208	2	0
4	A	3	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	4	0	0	0	0
4	D	1	0	0	0	0
4	F	1	0	0	0	0
4	H	4	0	0	0	0
All	All	5209	4415	4449	33	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 3.

All (33) 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:82:ARG:CB	1:A:82:ARG:CG	1.77	1.54
1:A:82:ARG:CG	1:A:82:ARG:CD	1.90	1.46
1:G:43:GLU:OE2	1:G:51:ARG:NE	2.07	0.88
1:H:81:PHE:C	1:H:82:ARG:HG3	2.02	0.79
1:H:81:PHE:O	1:H:82:ARG:HG3	1.88	0.74
1:B:55:LYS:NZ	1:B:61:ASP:O	2.25	0.69
1:B:112:GLU:OE1	1:B:112:GLU:N	2.25	0.64
1:B:39:GLY:HA3	1:B:53:PRO:HG3	1.78	0.64
1:A:82:ARG:HB3	1:A:85:ILE:HD13	1.83	0.60
2:C:1:DC:H2'	2:C:2:DA:C8	2.37	0.59
1:H:128:VAL:HG22	1:H:129:PRO:HD3	1.84	0.59
1:G:45:GLU:HA	1:G:45:GLU:OE1	2.03	0.59
1:G:61:ASP:OD1	1:G:61:ASP:N	2.39	0.56
1:A:85:ILE:HD12	1:A:85:ILE:N	2.25	0.52
3:F:2:DC:H2'	3:F:3:DT:H72	1.92	0.50
1:G:117:ASP:OD2	1:G:117:ASP:N	2.45	0.49
1:H:128:VAL:CG2	1:H:129:PRO:HD3	2.43	0.48
1:A:78:LYS:HE3	3:E:5:DT:OP1	2.14	0.47
2:C:4:DC:H2'	2:C:5:DT:H71	1.95	0.47
3:E:15:DA:H2''	3:E:16:DG:O5'	2.14	0.47
1:B:43:GLU:OE1	1:B:43:GLU:HA	2.14	0.47
2:C:11:DC:H2'	2:C:12:DG:C8	2.52	0.45
3:F:15:DA:H2''	3:F:16:DG:O5'	2.18	0.44
1:B:90:PRO:HA	1:B:93:TRP:CE3	2.52	0.44
1:A:90:PRO:N	1:A:91:PRO:CD	2.81	0.44
1:A:62:TYR:OH	2:D:9:DA:OP1	2.32	0.42
1:H:128:VAL:HG23	1:H:129:PRO:N	2.34	0.42
1:G:90:PRO:HA	1:G:93:TRP:CE3	2.55	0.42
1:A:44:ASN:ND2	1:A:46:GLU:HG2	2.35	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:13:DA:H2''	2:D:14:DG:C8	2.56	0.41
1:G:46:GLU:OE1	1:G:46:GLU:N	2.43	0.41
1:A:40:LEU:HD22	1:A:70:LEU:HD22	2.03	0.40
1:A:55:LYS:O	1:A:94:LYS:NZ	2.55	0.40

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:B:64:ARG:NH2	1:H:115:GLN:OE1[6_554]	1.94	0.26

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	106/111 (96%)	103 (97%)	3 (3%)	0	100	100
1	B	107/111 (96%)	103 (96%)	4 (4%)	0	100	100
1	G	107/111 (96%)	103 (96%)	4 (4%)	0	100	100
1	H	107/111 (96%)	102 (95%)	5 (5%)	0	100	100
All	All	427/444 (96%)	411 (96%)	16 (4%)	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	96/98 (98%)	95 (99%)	1 (1%)	76	89
1	B	97/98 (99%)	95 (98%)	2 (2%)	53	76
1	G	97/98 (99%)	92 (95%)	5 (5%)	23	41
1	H	97/98 (99%)	93 (96%)	4 (4%)	30	53
All	All	387/392 (99%)	375 (97%)	12 (3%)	40	64

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	82	ARG
1	B	64	ARG
1	B	120	ASP
1	G	21	ASN
1	G	45	GLU
1	G	46	GLU
1	G	51	ARG
1	G	64	ARG
1	H	60	GLN
1	H	87	LYS
1	H	119	SER
1	H	120	ASP

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

Mol	Chain	Res	Type
1	G	63	ASN

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 monosaccharides 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, 95th 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 ²)	Q < 0.9
1	A	108/111 (97%)	0.26	1 (0%) 84 86	48, 68, 96, 109	0
1	B	109/111 (98%)	0.37	2 (1%) 68 70	39, 51, 82, 98	0
1	G	109/111 (98%)	0.67	12 (11%) 5 5	43, 71, 111, 132	0
1	H	109/111 (98%)	0.30	4 (3%) 41 44	43, 62, 103, 119	0
2	C	19/19 (100%)	-0.03	0 100 100	47, 61, 89, 103	0
2	D	19/19 (100%)	0.00	1 (5%) 26 27	45, 52, 93, 96	0
3	E	19/19 (100%)	-0.12	0 100 100	41, 56, 95, 99	0
3	F	18/19 (94%)	-0.18	0 100 100	44, 63, 74, 94	0
All	All	510/520 (98%)	0.33	20 (3%) 39 41	39, 62, 103, 132	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	60	GLN	3.7
1	G	64	ARG	3.5
1	G	45	GLU	3.3
1	H	129	PRO	3.3
1	G	51	ARG	3.2
1	B	60	GLN	3.1
1	A	22	GLY	3.1
1	G	117	ASP	3.0
1	G	126	ARG	2.9
1	G	129	PRO	2.9
1	G	119	SER	2.8
1	G	59	ARG	2.7
1	H	21	ASN	2.7
2	D	1	DC	2.6
1	H	22	GLY	2.4
1	H	127	ILE	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	G	128	VAL	2.4
1	B	64	ARG	2.3
1	G	58	GLY	2.2
1	G	49	ILE	2.2

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.