



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 04:47 PM GMT

PDB ID : 4G8E  
Title : Crystal Structure of clone18 TCR  
Authors : Gras, S.; Bhati, M.; Rossjohn, J.  
Deposited on : 2012-07-23  
Resolution : 2.20 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](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

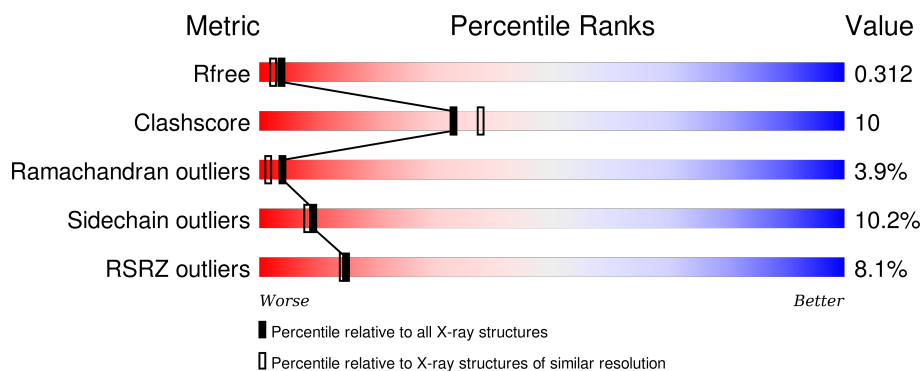
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

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	201	<div> <div>12%</div> <div>69%</div> <div>26%</div> <div>.</div> </div>
2	B	247	<div> <div>5%</div> <div>70%</div> <div>23%</div> <div>...</div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3625 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 alpha chain clone 18 TCR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	201	Total	C	N	O	S	0	0	0
			1566	987	256	314	9			

- Molecule 2 is a protein called beta chain clone 18 TCR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	241	Total	C	N	O	S	2	0	0
			1913	1210	331	363	9			

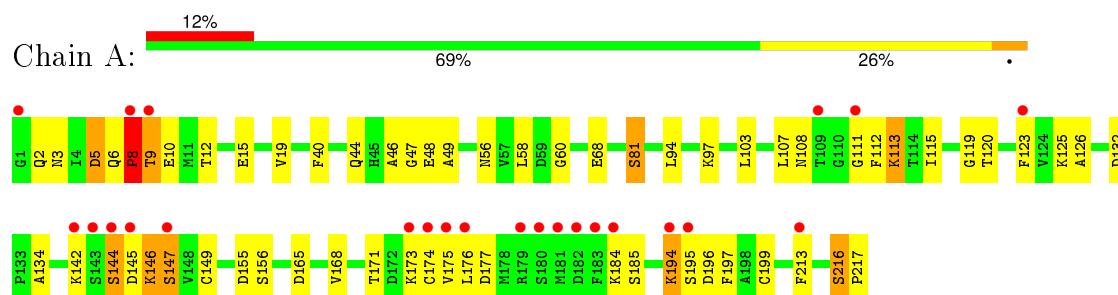
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	76	Total	O	0	0
			76	76		
3	B	70	Total	O	0	0
			70	70		

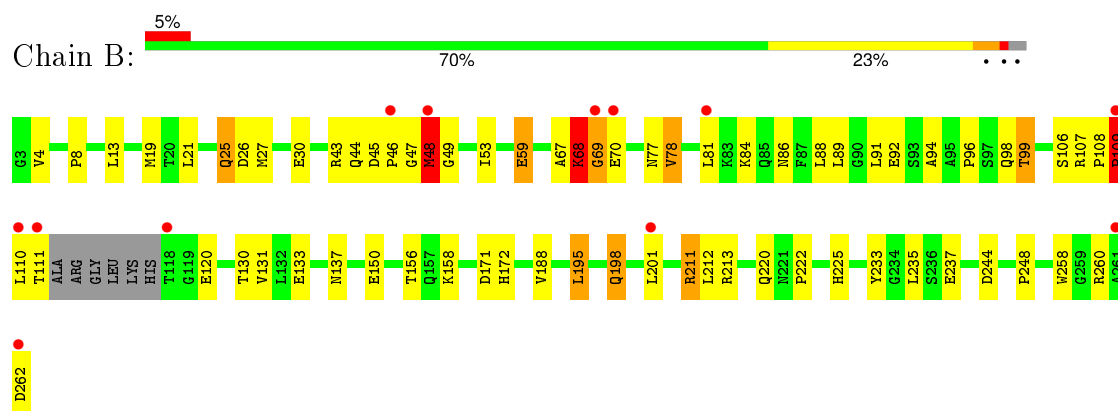
### 3 Residue-property plots [i](#)

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 ( $\text{RSRZ} > 2$ ). 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: alpha chain clone 18 TCR



- Molecule 2: beta chain clone 18 TCR



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	46.42Å 84.09Å 58.28Å 90.00° 111.88° 90.00°	Depositor
Resolution (Å)	45.48 – 2.20 45.49 – 2.20	Depositor EDS
% Data completeness (in resolution range)	97.6 (45.48-2.20) 97.6 (45.49-2.20)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.19 (at 2.20Å)	Xtriage
Refinement program	BUSTER 2.10.0	Depositor
R, $R_{free}$	0.241 , 0.293 0.250 , 0.312	Depositor DCC
$R_{free}$ test set	1062 reflections (5.42%)	DCC
Wilson B-factor (Å <sup>2</sup> )	25.0	Xtriage
Anisotropy	0.465	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.25 , 48.4	EDS
Estimated twinning fraction	0.032 for h,-k,-h-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 20661 reflections	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	3625	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.06% 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 [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	0.52	0/1600	0.91	1/2165 (0.0%)
2	B	0.50	0/1964	0.82	3/2669 (0.1%)
All	All	0.51	0/3564	0.86	4/4834 (0.1%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	8	PRO	N-CA-C	7.30	131.07	112.10
2	B	67	ALA	C-N-CA	6.19	137.17	121.70
2	B	47	GLY	C-N-CA	5.24	134.79	121.70
2	B	68	LYS	N-CA-C	5.10	124.78	111.00

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	1566	0	1493	34	0
2	B	1913	0	1835	40	0
3	A	76	0	0	0	0
3	B	70	0	0	0	0
All	All	3625	0	3328	70	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.

All (70) 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)
2:B:48:MET:HB2	2:B:49:GLY:CA	1.82	1.08
2:B:48:MET:CB	2:B:49:GLY:HA2	1.88	1.03
2:B:48:MET:HB2	2:B:49:GLY:HA2	1.05	1.02
2:B:96:PRO:O	2:B:99:THR:HG23	1.80	0.81
1:A:149:CYS:HG	1:A:199:CYS:HG	0.81	0.81
1:A:44:GLN:HE22	2:B:44:GLN:HE22	1.29	0.79
1:A:56:ASN:HD21	1:A:81:SER:HB3	1.49	0.76
1:A:8:PRO:HG3	1:A:119:GLY:O	1.90	0.71
1:A:40:PHE:HE2	1:A:107:LEU:HB2	1.58	0.69
1:A:10:GLU:HG2	1:A:123:PHE:CE2	2.26	0.68
2:B:8:PRO:HD2	2:B:21:LEU:HD23	1.75	0.68
2:B:198:GLN:HB3	2:B:201:LEU:HD13	1.79	0.64
2:B:109:PRO:HA	2:B:111:THR:H	1.63	0.63
1:A:15:GLU:O	1:A:94:LEU:O	2.18	0.61
2:B:45:ASP:O	2:B:48:MET:HB3	2.01	0.60
2:B:99:THR:HB	2:B:130:THR:HA	1.83	0.60
1:A:10:GLU:HG2	1:A:123:PHE:HE2	1.65	0.60
2:B:46:PRO:C	2:B:48:MET:H	2.06	0.58
2:B:13:LEU:HD11	2:B:19:MET:HG2	1.85	0.57
2:B:107:ARG:HE	2:B:109:PRO:HG2	1.70	0.57
2:B:188:VAL:HG12	2:B:212:LEU:HD13	1.87	0.56
2:B:108:PRO:HD2	2:B:109:PRO:HD3	1.86	0.56
1:A:111:GLY:O	1:A:113:LYS:N	2.38	0.56
1:A:8:PRO:HA	1:A:9:THR:C	2.17	0.56
2:B:99:THR:HG22	2:B:131:VAL:H	1.70	0.55
1:A:8:PRO:HD3	1:A:120:THR:HA	1.88	0.55
1:A:165:ASP:HB3	1:A:168:VAL:HG12	1.88	0.55
2:B:109:PRO:HA	2:B:111:THR:N	2.22	0.54
1:A:12:THR:HG22	1:A:123:PHE:HD2	1.72	0.53
1:A:176:LEU:HD22	2:B:213:ARG:HB2	1.91	0.53
2:B:94:ALA:HA	2:B:98:GLN:NE2	2.25	0.52
1:A:5:ASP:C	1:A:8:PRO:HD2	2.31	0.51
1:A:40:PHE:CE2	1:A:107:LEU:HB2	2.43	0.51
1:A:126:ALA:HB2	1:A:175:VAL:HG11	1.93	0.50
1:A:5:ASP:HB3	1:A:8:PRO:HD2	1.93	0.50
2:B:25:GLN:HG2	2:B:27:MET:H	1.76	0.49
2:B:13:LEU:HD21	2:B:19:MET:HB3	1.95	0.49
1:A:216:SER:H	1:A:217:PRO:HD2	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:6:GLN:N	1:A:8:PRO:HD2	2.28	0.48
2:B:99:THR:CG2	2:B:131:VAL:H	2.27	0.48
2:B:94:ALA:HA	2:B:98:GLN:HE22	1.79	0.48
2:B:21:LEU:HD12	2:B:89:LEU:HD23	1.95	0.47
1:A:56:ASN:ND2	1:A:81:SER:HB3	2.25	0.47
2:B:225:HIS:HB2	2:B:258:TRP:CZ3	2.50	0.47
1:A:175:VAL:HA	1:A:185:SER:O	2.14	0.47
2:B:30:GLU:HG2	2:B:84:LYS:HE3	1.96	0.46
1:A:144:SER:HB3	1:A:146:LYS:HE2	1.97	0.46
2:B:220:GLN:O	2:B:222:PRO:HD3	2.15	0.46
1:A:145:ASP:C	1:A:147:SER:H	2.19	0.46
1:A:176:LEU:HD21	2:B:211:ARG:HB2	1.98	0.45
2:B:69:GLY:HA3	2:B:70:GLU:HA	1.47	0.45
1:A:134:ALA:HB2	1:A:213:PHE:HB3	1.99	0.44
2:B:172:HIS:HB3	2:B:233:TYR:HB2	1.99	0.43
1:A:125:LYS:HD2	1:A:156:SER:HB3	2.00	0.43
2:B:235:LEU:HD22	2:B:248:PRO:HD2	1.99	0.43
1:A:46:ALA:HA	1:A:47:GLY:HA2	1.82	0.43
2:B:77:ASN:HD21	2:B:92:GLU:HG3	1.83	0.43
2:B:45:ASP:HB3	2:B:46:PRO:CD	2.49	0.43
2:B:48:MET:CG	2:B:49:GLY:HA2	2.46	0.42
1:A:12:THR:HG22	1:A:123:PHE:CD2	2.53	0.42
2:B:107:ARG:HG3	2:B:120:GLU:O	2.18	0.42
1:A:108:ASN:HD21	1:A:115:ILE:HD13	1.84	0.42
2:B:78:VAL:HA	2:B:88:LEU:O	2.21	0.41
1:A:195:SER:N	1:A:196:ASP:HA	2.36	0.41
2:B:43:ARG:HB3	2:B:53:ILE:HD11	2.03	0.41
1:A:177:ASP:HA	1:A:184:LYS:HA	2.03	0.41
1:A:48:GLU:HG3	1:A:49:ALA:H	1.84	0.41
2:B:220:GLN:HA	2:B:260:ARG:O	2.21	0.41
1:A:171:THR:HG22	2:B:195:LEU:HD13	2.02	0.40
2:B:156:THR:HB	2:B:158:LYS:HE2	2.04	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	199/201 (99%)	175 (88%)	13 (6%)	11 (6%)	2	1
2	B	237/247 (96%)	220 (93%)	11 (5%)	6 (2%)	7	3
All	All	436/448 (97%)	395 (91%)	24 (6%)	17 (4%)	4	1

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	GLN
1	A	8	PRO
1	A	112	PHE
1	A	147	SER
1	A	173	LYS
1	A	194	LYS
2	B	48	MET
2	B	68	LYS
1	A	142	LYS
1	A	146	LYS
1	A	216	SER
2	B	59	GLU
2	B	109	PRO
1	A	60	GLY
1	A	144	SER
2	B	171	ASP
2	B	69	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	175/175 (100%)	159 (91%)	16 (9%)	12	11
2	B	208/212 (98%)	185 (89%)	23 (11%)	8	6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	383/387 (99%)	344 (90%)	39 (10%)	<b>9</b> <b>8</b>

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ASN
1	A	5	ASP
1	A	8	PRO
1	A	9	THR
1	A	19	VAL
1	A	58	LEU
1	A	68	GLU
1	A	81	SER
1	A	97	LYS
1	A	103	LEU
1	A	113	LYS
1	A	132	ASP
1	A	155	ASP
1	A	174	CYS
1	A	194	LYS
1	A	197	PHE
2	B	4	VAL
2	B	25	GLN
2	B	26	ASP
2	B	48	MET
2	B	59	GLU
2	B	68	LYS
2	B	78	VAL
2	B	81	LEU
2	B	86	ASN
2	B	91	LEU
2	B	99	THR
2	B	106	SER
2	B	109	PRO
2	B	110	LEU
2	B	133	GLU
2	B	137	ASN
2	B	150	GLU
2	B	195	LEU
2	B	198	GLN
2	B	211	ARG
2	B	237	GLU

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Mol	Chain	Res	Type
2	B	244	ASP
2	B	262	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	44	GLN
1	A	45	HIS
1	A	56	ASN
1	A	108	ASN
1	A	127	ASN
2	B	25	GLN
2	B	77	ASN
2	B	98	GLN
2	B	137	ASN
2	B	231	GLN
2	B	251	GLN

### 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 ⓘ

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	201/201 (100%)	0.69	24 (11%) 6 6	14, 39, 69, 83	12 (5%)
2	B	241/247 (97%)	0.13	12 (4%) 32 32	14, 31, 56, 81	2 (0%)
All	All	442/448 (98%)	0.38	36 (8%) 15 14	14, 34, 63, 83	14 (3%)

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	181	MET	7.5
1	A	176	LEU	7.0
1	A	182	ASP	6.9
2	B	110	LEU	6.6
1	A	183	PHE	6.2
1	A	195	SER	6.1
1	A	8	PRO	5.2
1	A	180	SER	4.6
1	A	174	CYS	4.1
1	A	143	SER	3.9
2	B	118	THR	3.9
1	A	175	VAL	3.9
1	A	144	SER	3.6
1	A	184	LYS	3.5
1	A	145	ASP	3.4
1	A	9	THR	3.3
2	B	48	MET	3.3
2	B	261	ALA	3.1
2	B	81	LEU	3.1
1	A	142	LYS	3.0
2	B	46	PRO	3.0
2	B	111	THR	3.0
1	A	111	GLY	2.9
2	B	262	ASP	2.9

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Mol	Chain	Res	Type	RSRZ
2	B	109	PRO	2.7
1	A	147	SER	2.7
1	A	123	PHE	2.6
1	A	173	LYS	2.5
2	B	70	GLU	2.5
1	A	179	ARG	2.4
1	A	1	GLY	2.4
1	A	213	PHE	2.4
2	B	69	GLY	2.3
2	B	201	LEU	2.1
1	A	109	THR	2.0
1	A	194	LYS	2.0

## 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 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.