



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 11:56 AM GMT

PDB ID : 3QEQ
Title : The complex between TCR DMF4 and human Class I MHC HLA-A2 with the bound MART-1(27-35) nonameric peptide
Authors : Borbulevych, O.Y.; Baker, B.M.
Deposited on : 2011-01-20
Resolution : 2.59 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
<http://wwpdb.org/validation/2016/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
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

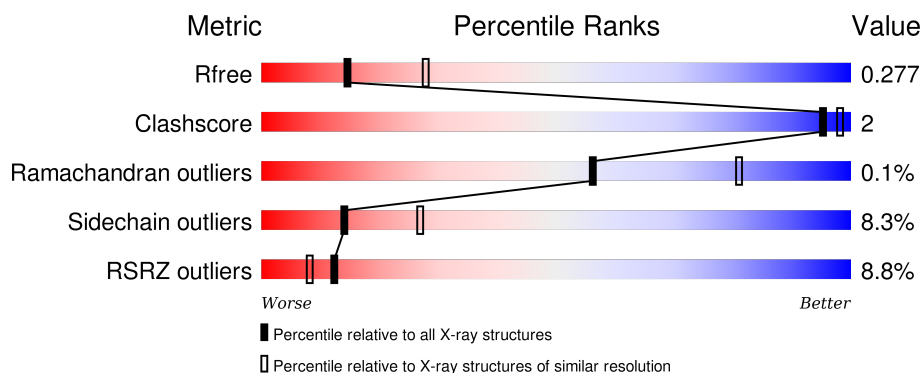
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.59 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	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)

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 ≥ 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	275	<div> <div>6%</div> <div>88%</div> <div>12%</div> </div>
2	B	100	<div> <div>7%</div> <div>91%</div> <div>9%</div> </div>
3	C	9	<div> <div>11%</div> <div>89%</div> <div>11%</div> </div>
4	D	194	<div> <div>15%</div> <div>85%</div> <div>14%</div> <div>•</div> </div>
5	E	243	<div> <div>7%</div> <div>89%</div> <div>10%</div> <div>•</div> </div>

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 6679 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 HLA class I histocompatibility antigen, A-2 alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	275	Total	C	N	O	S	0	0	0
			2247	1403	409	426	9			

- Molecule 2 is a protein called Beta-2-microglobulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	100	Total	C	N	O	S	0	0	0
			837	533	141	159	4			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	MET	-	INITIATING METHIONINE	UNP P61769

- Molecule 3 is a protein called MART-1(27-35) peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	9	Total	C	N	O	0	0	0
			57	37	9	11			

- Molecule 4 is a protein called DMF4 alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	194	Total	C	N	O	S	0	0	0
			1497	938	243	307	9			

- Molecule 5 is a protein called DMF4 beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	243	Total	C	N	O	S	0	0	0
			1938	1213	340	379	6			

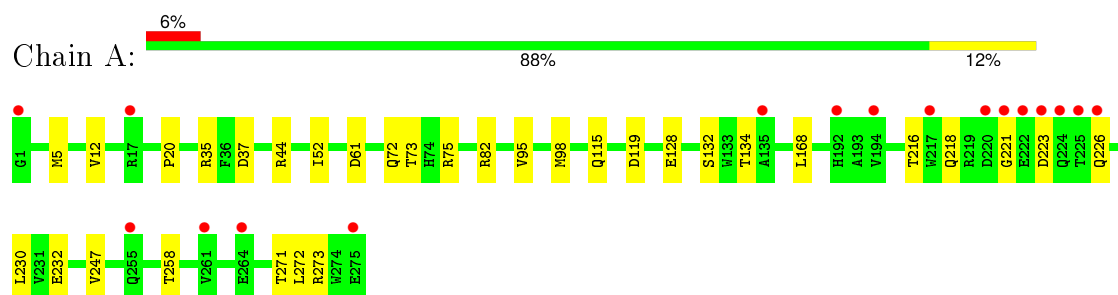
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	39	Total 39	O 39	0	0
6	B	9	Total 9	O 9	0	0
6	C	1	Total 1	O 1	0	0
6	D	16	Total 16	O 16	0	0
6	E	38	Total 38	O 38	0	0

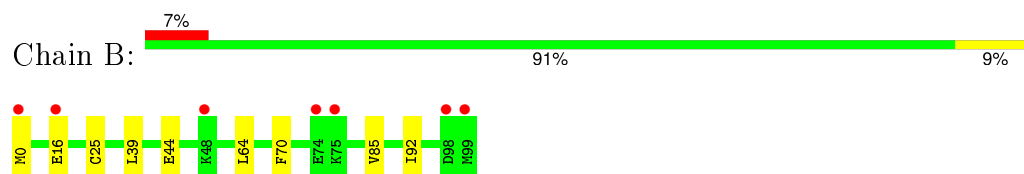
3 Residue-property plots [i](#)

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 ($RSRZ > 2$). 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.

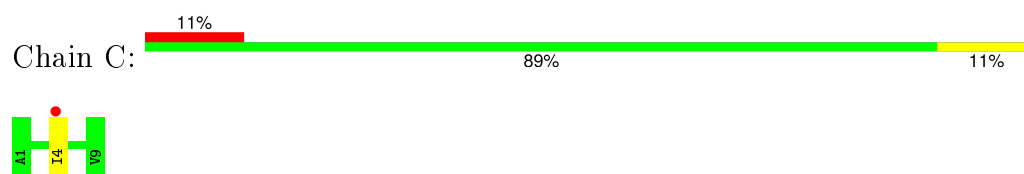
- Molecule 1: HLA class I histocompatibility antigen, A-2 alpha chain



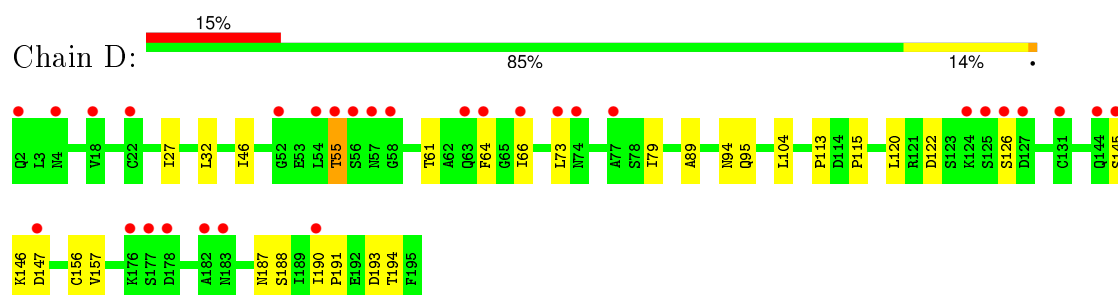
- Molecule 2: Beta-2-microglobulin



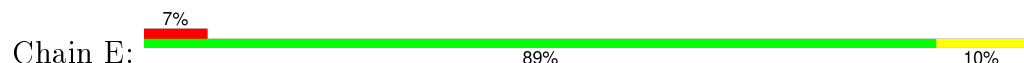
- Molecule 3: MART-1(27-35) peptide

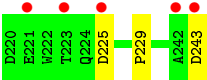
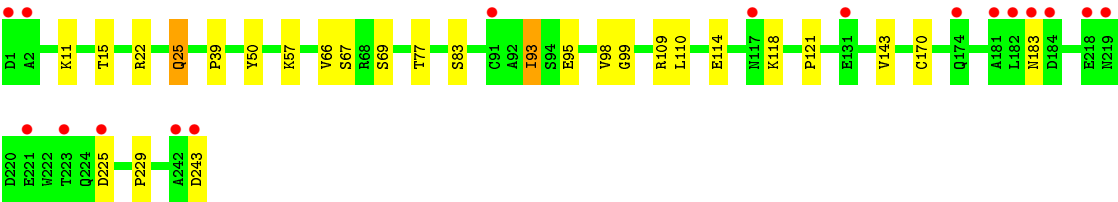


- Molecule 4: DMF4 alpha chain



- Molecule 5: DMF4 beta chain





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	59.65Å 73.66Å 225.29Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.59 19.81 – 2.59	Depositor EDS
% Data completeness (in resolution range)	99.1 (20.00-2.59) 99.1 (19.81-2.59)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.34 (at 2.59Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.215 , 0.269 0.223 , 0.277	Depositor DCC
R_{free} test set	1602 reflections (5.35%)	DCC
Wilson B-factor (Å ²)	38.1	Xtriage
Anisotropy	0.115	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 49.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 31550 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	6679	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.46% 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, 0.375 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	0.60	0/2312	0.76	1/3137 (0.0%)
2	B	0.58	0/860	0.67	0/1162
3	C	0.97	0/56	1.02	0/74
4	D	0.62	0/1529	0.84	4/2074 (0.2%)
5	E	0.60	0/1991	0.80	0/2710
All	All	0.61	0/6748	0.78	5/9157 (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
4	D	0	1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	156	CYS	CA-CB-SG	6.79	126.23	114.00
4	D	120	LEU	CA-CB-CG	6.18	129.52	115.30
1	A	37	ASP	CB-CG-OD1	5.26	123.03	118.30
4	D	120	LEU	CB-CG-CD1	-5.13	102.28	111.00
4	D	122	ASP	CB-CG-OD1	5.04	122.84	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	D	113	PRO	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	2247	0	2096	8	0
2	B	837	0	803	2	0
3	C	57	0	67	2	0
4	D	1497	0	1413	6	0
5	E	1938	0	1826	7	0
6	A	39	0	0	0	0
6	B	9	0	0	0	0
6	C	1	0	0	0	0
6	D	16	0	0	0	0
6	E	38	0	0	0	0
All	All	6679	0	6205	20	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 2.

All (20) 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)
3:C:4:ILE:HG22	5:E:99:GLY:HA3	1.89	0.53
1:A:72:GLN:HG3	5:E:50:TYR:HB3	1.93	0.50
5:E:121:PRO:HD3	5:E:229:PRO:HB3	1.95	0.48
4:D:32:LEU:HB2	4:D:89:ALA:HB3	1.97	0.47
1:A:44:ARG:NH2	1:A:61:ASP:OD1	2.48	0.47
1:A:20:PRO:HG2	1:A:75:ARG:HG2	1.97	0.45
3:C:4:ILE:HG23	5:E:98:VAL:HG12	1.99	0.45
1:A:218:GLN:HA	1:A:223:ASP:HA	1.97	0.45
2:B:25:CYS:HB2	2:B:39:LEU:HD21	1.99	0.44
1:A:218:GLN:HE21	1:A:221:GLY:HA2	1.83	0.44
1:A:258:THR:HG22	1:A:273:ARG:HB3	1.99	0.44
4:D:115:PRO:HG2	4:D:193:ASP:HB3	1.99	0.43
1:A:5:MET:HB2	1:A:168:LEU:HD13	2.02	0.42
4:D:94:ASN:ND2	5:E:50:TYR:OH	2.52	0.42
5:E:11:LYS:HB3	5:E:110:LEU:HD13	2.02	0.42
4:D:55:THR:HB	4:D:61:THR:HG22	2.02	0.41
5:E:25:GLN:HG3	5:E:93:ILE:HG12	2.01	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:190:ILE:H	4:D:190:ILE:HG13	1.46	0.41
4:D:146:LYS:HB3	4:D:147:ASP:H	1.61	0.41
1:A:119:ASP:HB3	2:B:0:MET:HA	2.03	0.41

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	273/275 (99%)	269 (98%)	4 (2%)	0	100	100
2	B	98/100 (98%)	96 (98%)	2 (2%)	0	100	100
3	C	7/9 (78%)	5 (71%)	2 (29%)	0	100	100
4	D	192/194 (99%)	177 (92%)	14 (7%)	1 (0%)	34	60
5	E	241/243 (99%)	231 (96%)	10 (4%)	0	100	100
All	All	811/821 (99%)	778 (96%)	32 (4%)	1 (0%)	56	81

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	191	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	
1	A	231/231 (100%)	213 (92%)	18 (8%)	16	30
2	B	95/95 (100%)	89 (94%)	6 (6%)	22	44
3	C	5/5 (100%)	5 (100%)	0	100	100
4	D	171/171 (100%)	156 (91%)	15 (9%)	12	24
5	E	213/213 (100%)	193 (91%)	20 (9%)	11	20
All	All	715/715 (100%)	656 (92%)	59 (8%)	14	27

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	VAL
1	A	35	ARG
1	A	52	ILE
1	A	73	THR
1	A	82	ARG
1	A	95	VAL
1	A	98	MET
1	A	115	GLN
1	A	128	GLU
1	A	132	SER
1	A	134	THR
1	A	216	THR
1	A	226	GLN
1	A	230	LEU
1	A	232	GLU
1	A	247	VAL
1	A	271	THR
1	A	272	LEU
2	B	16	GLU
2	B	44	GLU
2	B	64	LEU
2	B	70	PHE
2	B	85	VAL
2	B	92	ILE
4	D	27	ILE
4	D	46	ILE
4	D	55	THR
4	D	64	PHE
4	D	66	ILE
4	D	73	LEU
4	D	79	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	D	95	GLN
4	D	104	LEU
4	D	126	SER
4	D	145	SER
4	D	157	VAL
4	D	187	ASN
4	D	188	SER
4	D	194	THR
5	E	15	THR
5	E	22	ARG
5	E	25	GLN
5	E	39	PRO
5	E	57	LYS
5	E	66	VAL
5	E	67	SER
5	E	69	SER
5	E	77	THR
5	E	83	SER
5	E	93	ILE
5	E	95	GLU
5	E	109	ARG
5	E	114	GLU
5	E	118	LYS
5	E	143	VAL
5	E	170	CYS
5	E	183	ASN
5	E	225	ASP
5	E	243	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	218	GLN
4	D	5	GLN
4	D	13	GLN
4	D	175	ASN

5.3.3 RNA ⓘ

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

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	275/275 (100%)	0.38	17 (6%) 24 18	27, 50, 99, 129	0
2	B	100/100 (100%)	0.55	7 (7%) 19 13	30, 56, 98, 111	0
3	C	9/9 (100%)	1.31	1 (11%) 7 4	34, 38, 44, 47	0
4	D	194/194 (100%)	0.96	30 (15%) 3 1	30, 73, 115, 139	0
5	E	243/243 (100%)	0.30	17 (6%) 19 13	27, 47, 78, 99	0
All	All	821/821 (100%)	0.53	72 (8%) 12 8	27, 52, 102, 139	0

All (72) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	D	56	SER	7.8
2	B	99	MET	7.1
4	D	2	GLN	6.5
5	E	243	ASP	6.4
4	D	127	ASP	5.2
4	D	126	SER	5.0
1	A	221	GLY	4.7
2	B	0	MET	4.7
4	D	176	LYS	4.6
5	E	1	ASP	4.2
1	A	220	ASP	4.2
3	C	4	ILE	4.1
1	A	1	GLY	4.0
4	D	57	ASN	4.0
1	A	226	GLN	4.0
1	A	224	GLN	3.8
4	D	177	SER	3.8
1	A	223	ASP	3.8
4	D	18	VAL	3.4
4	D	66	ILE	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	16	GLU	3.3
1	A	222	GLU	3.3
1	A	275	GLU	3.2
5	E	225	ASP	3.1
5	E	183	ASN	3.1
5	E	223	THR	3.1
5	E	117	ASN	3.1
1	A	225	THR	3.0
5	E	184	ASP	3.0
4	D	74	ASN	2.9
4	D	54	LEU	2.9
4	D	77	ALA	2.9
4	D	125	SER	2.8
2	B	75	LYS	2.8
4	D	145	SER	2.8
4	D	52	GLY	2.7
4	D	64	PHE	2.7
5	E	181	ALA	2.7
4	D	73	LEU	2.7
4	D	178	ASP	2.6
4	D	147	ASP	2.5
4	D	22	CYS	2.5
2	B	48	LYS	2.4
4	D	4	ASN	2.4
2	B	98	ASP	2.4
1	A	255	GLN	2.4
5	E	174	GLN	2.3
1	A	192	HIS	2.3
4	D	124	LYS	2.3
5	E	219	ASN	2.3
1	A	17	ARG	2.3
1	A	264	GLU	2.2
4	D	190	ILE	2.2
1	A	194	VAL	2.2
1	A	135	ALA	2.2
4	D	55	THR	2.2
5	E	218	GLU	2.2
5	E	131	GLU	2.2
1	A	261	VAL	2.2
4	D	183	ASN	2.2
2	B	74	GLU	2.2
4	D	131	CYS	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
5	E	2	ALA	2.1
4	D	144	GLN	2.1
5	E	182	LEU	2.1
4	D	58	GLY	2.1
1	A	217	TRP	2.1
5	E	91	CYS	2.1
4	D	182	ALA	2.0
5	E	242	ALA	2.0
4	D	63	GLN	2.0
5	E	221	GLU	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.