



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 24, 2024 – 03:43 PM EDT

PDB ID : 6AM5
Title : Crystal structure of DMF5 TCR bound to HLA-A2 presenting synthetic peptide SMLGIGIVPV
Authors : Riley, T.P.; Baker, B.M.
Deposited on : 2017-08-09
Resolution : 2.39 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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	:	2.37.1
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)	:	2.37.1

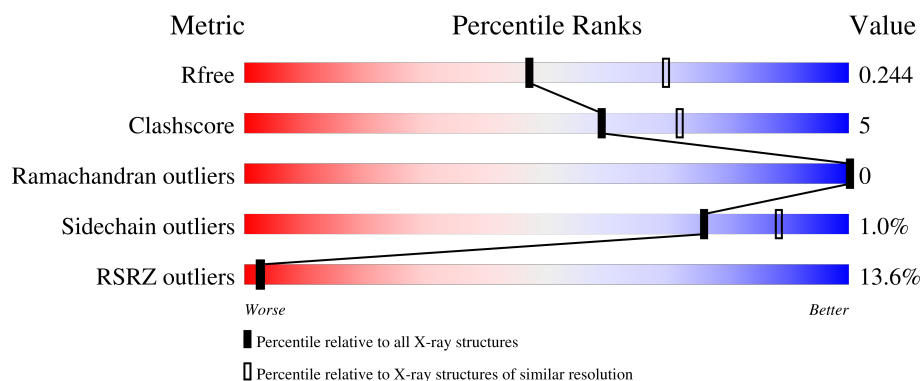
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.39 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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	275	<div> <div>13%</div> <div>88%</div> <div>11%</div> </div>
2	B	100	<div> <div>90%</div> <div>10%</div> </div>
3	C	10	<div> <div>100%</div> </div>
4	D	189	<div> <div>23%</div> <div>91%</div> <div>9%</div> </div>
5	E	242	<div> <div>13%</div> <div>85%</div> <div>15%</div> </div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 6696 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	1	MET	-	initiating methionine	UNP P61769

- Molecule 3 is a protein called SER-MET-LEU-GLY-ILE-GLY-ILE-VAL-PRO-VAL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	10	Total	C	N	O	S	0	0	0
			68	45	10	12	1			

- Molecule 4 is a protein called DMF5 TCR alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	189	Total	C	N	O	S	0	0	0
			1455	907	241	299	8			

- Molecule 5 is a protein called DMF5 TCR beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	242	Total	C	N	O	S	0	0	0
			1877	1181	330	358	8			

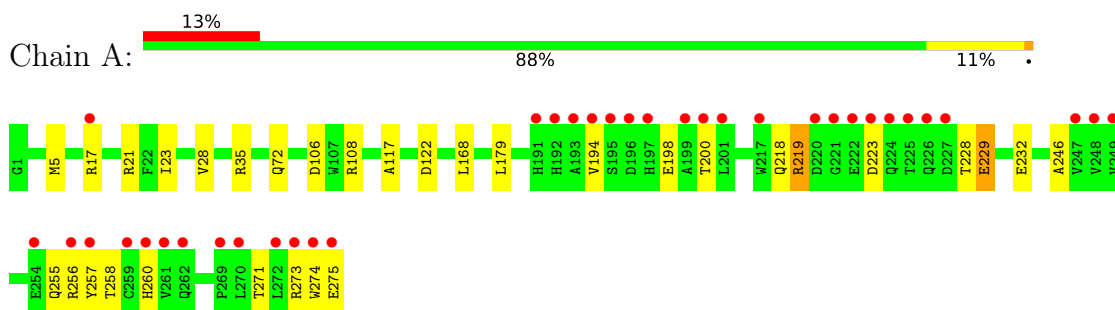
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	97	Total 97	O 97	0	0
6	B	41	Total 41	O 41	0	0
6	C	5	Total 5	O 5	0	0
6	D	29	Total 29	O 29	0	0
6	E	40	Total 40	O 40	0	0

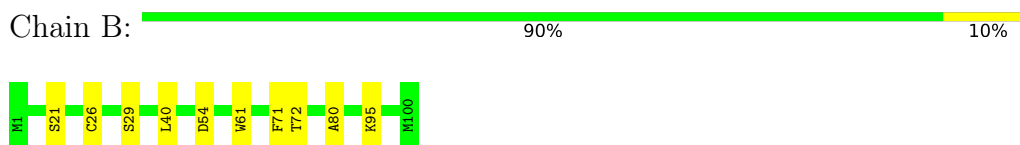
3 Residue-property plots [i](#)

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



- Molecule 2: Beta-2-microglobulin

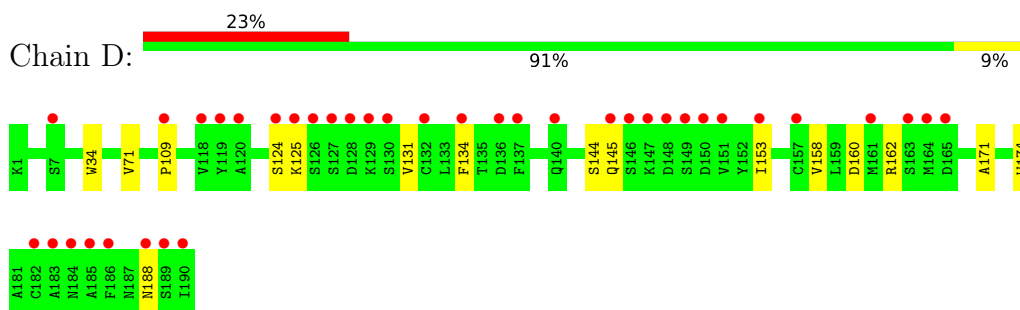


- Molecule 3: SER-MET-LEU-GLY-ILE-GLY-ILE-VAL-PRO-VAL

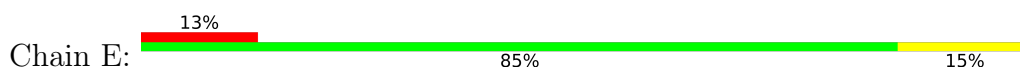


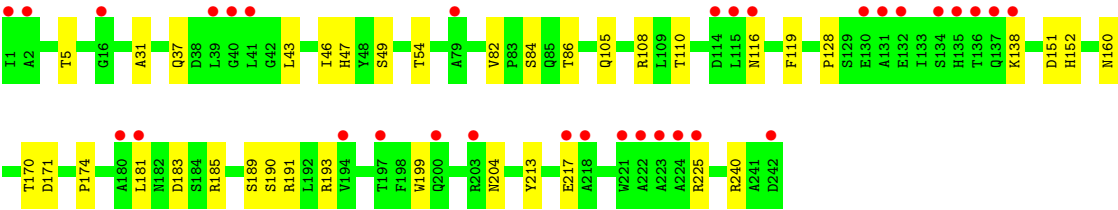
There are no outlier residues recorded for this chain.

- Molecule 4: DMF5 TCR alpha chain



- Molecule 5: DMF5 TCR beta chain





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	228.11Å 49.90Å 92.45Å 90.00° 95.72° 90.00°	Depositor
Resolution (Å)	38.75 – 2.39 38.75 – 2.39	Depositor EDS
% Data completeness (in resolution range)	93.6 (38.75-2.39) 93.2 (38.75-2.39)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.12 (at 2.39Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.201 , 0.244 0.201 , 0.244	Depositor DCC
R_{free} test set	2000 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	23.9	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 50.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	6696	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.93% 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 [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	0.27	0/2312	0.46	0/3137
2	B	0.23	0/860	0.41	0/1162
3	C	0.21	0/68	0.46	0/90
4	D	0.25	0/1484	0.48	0/2007
5	E	0.25	0/1926	0.44	0/2626
All	All	0.25	0/6650	0.45	0/9022

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	2247	0	2096	23	0
2	B	837	0	803	7	0
3	C	68	0	80	0	0
4	D	1455	0	1376	15	0
5	E	1877	0	1797	19	0
6	A	97	0	0	1	0
6	B	41	0	0	0	0
6	C	5	0	0	0	0
6	D	29	0	0	0	0
6	E	40	0	0	0	0
All	All	6696	0	6152	59	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 5.

All (59) 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:228:THR:HG23	1:A:246:ALA:O	1.80	0.80
2:B:80:ALA:HB2	2:B:95:LYS:HD2	1.70	0.74
4:D:134:PHE:HB2	4:D:171:ALA:HB3	1.70	0.73
1:A:219:ARG:NH1	1:A:256:ARG:HD3	2.05	0.72
5:E:116:ASN:O	5:E:225:ARG:NH1	2.30	0.65
5:E:151:ASP:HB2	5:E:174:PRO:HG2	1.83	0.61
5:E:170:THR:HG23	5:E:190:SER:HB2	1.83	0.61
5:E:37:GLN:HB2	5:E:43:LEU:HD23	1.83	0.60
1:A:194:VAL:HG22	1:A:200:THR:HG23	1.84	0.59
1:A:35:ARG:HD3	2:B:54:ASP:OD2	2.03	0.58
4:D:124:SER:O	4:D:125:LYS:HB2	2.04	0.58
1:A:218:GLN:HG2	1:A:223:ASP:HA	1.87	0.56
1:A:260:HIS:HD1	1:A:271:THR:HG22	1.69	0.56
1:A:122:ASP:OD1	2:B:61:TRP:NE1	2.36	0.56
4:D:34:TRP:HE1	4:D:71:VAL:HG22	1.73	0.54
1:A:72:GLN:HG2	5:E:54:THR:HG21	1.90	0.54
1:A:5:MET:HB2	1:A:168:LEU:HD13	1.91	0.52
5:E:138:LYS:HB3	5:E:193:ARG:HE	1.75	0.51
1:A:228:THR:HG22	1:A:229:GLU:N	2.25	0.51
4:D:160:ASP:OD2	4:D:162:ARG:HG2	2.10	0.51
5:E:171:ASP:OD2	5:E:189:SER:HB3	2.11	0.51
5:E:86:THR:HG23	5:E:110:THR:HA	1.96	0.48
1:A:194:VAL:CG2	1:A:200:THR:HG23	2.45	0.47
2:B:21:SER:HA	2:B:72:THR:HG22	1.96	0.47
1:A:232:GLU:OE1	2:B:29:SER:OG	2.29	0.46
1:A:28:VAL:HG11	1:A:179:LEU:HD13	1.98	0.46
5:E:5:THR:HG23	5:E:105:GLN:HE22	1.81	0.46
4:D:145:GLN:CB	4:D:153:ILE:HB	2.46	0.46
4:D:144:SER:H	4:D:188:ASN:ND2	2.14	0.46
5:E:128:PRO:HD2	5:E:199:TRP:CZ2	2.51	0.46
1:A:228:THR:CG2	1:A:229:GLU:N	2.78	0.45
4:D:109:PRO:HG3	4:D:158:VAL:HG11	1.99	0.45
4:D:131:VAL:HG12	4:D:174:TRP:HB3	1.98	0.45
1:A:106:ASP:OD2	1:A:108:ARG:NH1	2.50	0.45
4:D:145:GLN:HB3	4:D:153:ILE:HB	1.98	0.45
5:E:82:VAL:HG12	5:E:84:SER:H	1.82	0.45
1:A:194:VAL:HG22	1:A:200:THR:CG2	2.45	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:258:THR:HG22	1:A:273:ARG:HG3	1.99	0.45
1:A:17:ARG:NH1	6:A:309:HOH:O	2.50	0.44
1:A:274:TRP:CD1	1:A:275:GLU:HG3	2.53	0.44
4:D:144:SER:H	4:D:188:ASN:HD21	1.65	0.44
5:E:31:ALA:HA	5:E:49:SER:O	2.18	0.44
4:D:145:GLN:HA	4:D:153:ILE:HD12	2.00	0.43
4:D:134:PHE:O	4:D:171:ALA:N	2.51	0.43
4:D:124:SER:O	4:D:125:LYS:CB	2.67	0.43
5:E:160:ASN:ND2	5:E:204:ASN:OD1	2.52	0.43
4:D:179:ASP:N	4:D:179:ASP:OD1	2.51	0.43
5:E:46:ILE:HG22	5:E:47:HIS:CD2	2.54	0.43
1:A:117:ALA:HB2	2:B:61:TRP:CE2	2.55	0.42
4:D:144:SER:N	4:D:188:ASN:OD1	2.52	0.42
5:E:119:PHE:CE1	5:E:185:ARG:NH1	2.87	0.42
5:E:152:HIS:HB3	5:E:213:TYR:HB2	2.01	0.42
2:B:26:CYS:HB2	2:B:40:LEU:HD21	2.02	0.42
1:A:21:ARG:CZ	1:A:23:ILE:HD11	2.50	0.42
5:E:181:LEU:HB3	5:E:183:ASP:OD1	2.20	0.41
1:A:219:ARG:HH11	1:A:256:ARG:HD3	1.81	0.41
5:E:217:GLU:N	5:E:217:GLU:OE1	2.54	0.41
5:E:108:ARG:HD2	5:E:152:HIS:CD2	2.56	0.41
1:A:219:ARG:HG3	1:A:257:TYR:CE2	2.56	0.40

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%)	261 (96%)	12 (4%)	0	100	100
2	B	98/100 (98%)	97 (99%)	1 (1%)	0	100	100
3	C	8/10 (80%)	8 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	D	187/189 (99%)	175 (94%)	12 (6%)	0	100	100
5	E	240/242 (99%)	230 (96%)	10 (4%)	0	100	100
All	All	806/816 (99%)	771 (96%)	35 (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	231/231 (100%)	227 (98%)	4 (2%)	60	78
2	B	95/95 (100%)	94 (99%)	1 (1%)	73	87
3	C	8/8 (100%)	8 (100%)	0	100	100
4	D	164/165 (99%)	164 (100%)	0	100	100
5	E	198/198 (100%)	196 (99%)	2 (1%)	76	88
All	All	696/697 (100%)	689 (99%)	7 (1%)	76	88

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	198	GLU
1	A	219	ARG
1	A	229	GLU
1	A	255	GLN
2	B	71	PHE
5	E	191	ARG
5	E	240	ARG

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

Mol	Chain	Res	Type
1	A	218	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 monosaccharides 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%)	0.54	36 (13%) 3 3	12, 37, 117, 166	0
2	B	100/100 (100%)	-0.17	0 100 100	18, 30, 69, 86	0
3	C	10/10 (100%)	0.47	0 100 100	15, 17, 23, 28	0
4	D	189/189 (100%)	1.20	43 (22%) 0 0	16, 55, 130, 145	0
5	E	242/242 (100%)	0.75	32 (13%) 3 3	13, 57, 103, 130	0
All	All	816/816 (100%)	0.67	111 (13%) 3 2	12, 44, 114, 166	0

All (111) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	194	VAL	7.8
4	D	149	SER	7.7
5	E	41	LEU	7.6
1	A	226	GLN	7.4
4	D	126	SER	7.1
4	D	176	ASN	7.1
4	D	180	PHE	6.5
4	D	147	LYS	6.3
5	E	224	ALA	6.0
5	E	131	ALA	5.6
1	A	200	THR	5.5
1	A	192	HIS	5.3
4	D	118	VAL	5.1
5	E	180	ALA	5.0
1	A	227	ASP	4.9
1	A	223	ASP	4.9
1	A	257	TYR	4.8
4	D	179	ASP	4.8
4	D	137	PHE	4.7
4	D	146	SER	4.6

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Mol	Chain	Res	Type	RSRZ
4	D	189	SER	4.6
5	E	218	ALA	4.5
4	D	148	ASP	4.4
4	D	175	SER	4.3
4	D	163	SER	4.3
4	D	164	MET	4.2
1	A	270	LEU	4.1
5	E	222	ALA	4.1
4	D	134	PHE	4.1
5	E	39	LEU	4.0
5	E	130	GLU	4.0
4	D	130	SER	3.9
1	A	224	GLN	3.9
1	A	269	PRO	3.9
1	A	193	ALA	3.8
4	D	184	ASN	3.8
4	D	177	LYS	3.8
4	D	182	CYS	3.7
5	E	115	LEU	3.7
4	D	186	PHE	3.6
5	E	197	THR	3.6
1	A	260	HIS	3.6
1	A	249	VAL	3.5
4	D	183	ALA	3.5
1	A	195	SER	3.5
4	D	151	VAL	3.5
1	A	197	HIS	3.5
4	D	157	CYS	3.4
1	A	225	THR	3.4
1	A	220	ASP	3.4
4	D	132	CYS	3.3
4	D	145	GLN	3.3
5	E	135	HIS	3.3
1	A	256	ARG	3.3
1	A	199	ALA	3.2
4	D	190	ILE	3.2
5	E	225	ARG	3.1
4	D	127	SER	3.1
5	E	223	ALA	3.1
4	D	150	ASP	3.1
4	D	140	GLN	3.0
4	D	128	ASP	3.0

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Mol	Chain	Res	Type	RSRZ
4	D	136	ASP	3.0
1	A	275	GLU	3.0
1	A	261	VAL	3.0
4	D	161	MET	2.9
5	E	1	ILE	2.8
4	D	124	SER	2.8
4	D	120	ALA	2.8
1	A	196	ASP	2.8
5	E	116	ASN	2.7
4	D	109	PRO	2.7
1	A	274	TRP	2.7
1	A	272	LEU	2.7
5	E	137	GLN	2.7
1	A	221	GLY	2.7
5	E	221	TRP	2.6
1	A	273	ARG	2.6
1	A	201	LEU	2.6
4	D	7	SER	2.5
4	D	125	LYS	2.5
4	D	119	TYR	2.5
1	A	222	GLU	2.5
5	E	114	ASP	2.4
1	A	191	HIS	2.4
5	E	79	ALA	2.4
4	D	153	ILE	2.4
4	D	165	ASP	2.4
5	E	136	THR	2.4
4	D	185	ALA	2.4
5	E	200	GLN	2.3
5	E	242	ASP	2.3
1	A	254	GLU	2.3
1	A	247	VAL	2.3
5	E	194	VAL	2.2
1	A	259	CYS	2.2
1	A	262	GLN	2.2
1	A	17	ARG	2.2
5	E	132	GLU	2.2
5	E	203	ARG	2.1
4	D	129	LYS	2.1
5	E	181	LEU	2.1
5	E	40	GLY	2.1
1	A	248	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
5	E	138	LYS	2.1
1	A	217	TRP	2.1
5	E	134	SER	2.1
5	E	217	GLU	2.0
4	D	188	ASN	2.0
5	E	16	GLY	2.0
5	E	2	ALA	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 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.