



Full wwPDB X-ray Structure Validation Report ⓘ

May 24, 2020 – 12:47 pm BST

PDB ID : 3VXQ
Title : H27-14 TCR specific for HLA-A24-Nef134-10
Authors : Shimizu, A.; Fukai, S.; Yamagata, A.; Iwamoto, A.
Deposited on : 2012-09-20
Resolution : 2.00 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
Xtrriage (Phenix) : 1.13
EDS : 2.11
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) : 2.11

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7672 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 H27-14 TCR alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	D	204	1575	978	266	323	8	0	0	0
1	A	204	1575	978	266	323	8	0	0	0

- Molecule 2 is a protein called H27-14 TCR beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	E	242	1954	1226	347	375	6	0	0	0
2	B	242	1954	1226	347	375	6	0	0	0

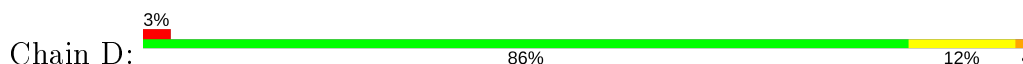
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	158	Total 158	O 158	0	0
3	E	185	Total 185	O 185	0	0
3	A	130	Total 130	O 130	0	0
3	B	141	Total 141	O 141	0	0

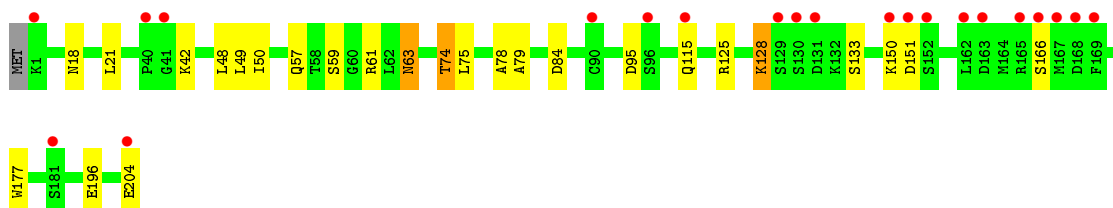
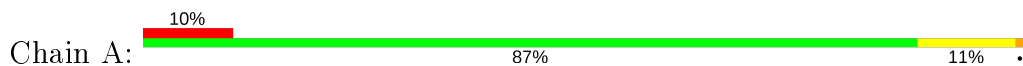
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

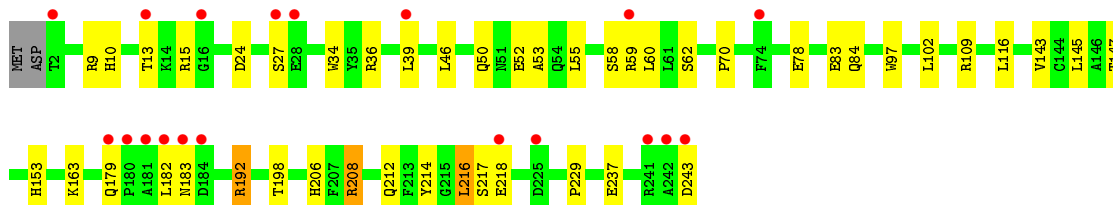
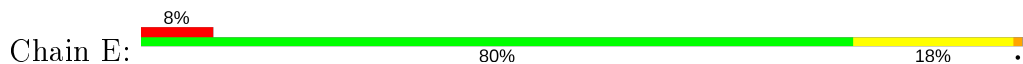
- Molecule 1: H27-14 TCR alpha chain



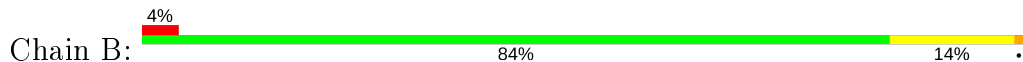
- Molecule 1: H27-14 TCR alpha chain

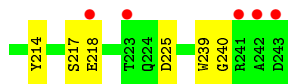


- Molecule 2: H27-14 TCR beta chain



- Molecule 2: H27-14 TCR beta chain





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	42.42Å 159.17Å 68.35Å 90.00° 93.56° 90.00°	Depositor
Resolution (Å)	50.00 – 2.00 27.41 – 2.00	Depositor EDS
% Data completeness (in resolution range)	97.8 (50.00-2.00) 97.9 (27.41-2.00)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.29 (at 1.99Å)	Xtrriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.222 , 0.267 0.222 , 0.268	Depositor DCC
R_{free} test set	3027 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	21.6	Xtrriage
Anisotropy	0.046	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 53.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	7672	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.04% 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	0.40	1/1604 (0.1%)	0.56	0/2175
1	D	0.40	1/1604 (0.1%)	0.58	0/2175
2	B	0.53	3/2006 (0.1%)	0.56	0/2724
2	E	0.53	1/2006 (0.0%)	0.59	0/2724
All	All	0.48	6/7220 (0.1%)	0.57	0/9798

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	34	TRP	CD2-CE2	5.26	1.47	1.41
1	D	35	TRP	CD2-CE2	5.12	1.47	1.41
2	E	97	TRP	CD2-CE2	5.09	1.47	1.41
1	A	177	TRP	CD2-CE2	5.08	1.47	1.41
2	B	97	TRP	CD2-CE2	5.08	1.47	1.41
2	B	239	TRP	CD2-CE2	5.05	1.47	1.41

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	1575	0	1522	18	0
1	D	1575	0	1522	21	0
2	B	1954	0	1850	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	1954	0	1850	33	0
3	A	130	0	0	7	0
3	B	141	0	0	5	0
3	D	158	0	0	4	0
3	E	185	0	0	16	0
All	All	7672	0	6744	85	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 6.

All (85) 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:D:202:SER:HB3	1:D:203:PRO:HD2	1.50	0.91
2:E:59:ARG:HH12	2:E:60:LEU:HB3	1.45	0.82
2:E:59:ARG:NH1	2:E:60:LEU:HB3	1.94	0.82
2:E:34:TRP:CZ2	3:E:474:HOH:O	2.32	0.81
1:D:41:GLY:HA3	3:D:368:HOH:O	1.88	0.72
1:D:13:VAL:HG21	1:D:19:LEU:HD22	1.72	0.72
1:D:202:SER:HB3	1:D:203:PRO:CD	2.25	0.67
2:E:34:TRP:HZ2	3:E:474:HOH:O	1.74	0.67
1:D:18:ASN:HD22	1:D:79:ALA:H	1.43	0.67
2:B:179:GLN:HG3	3:B:433:HOH:O	1.96	0.65
2:E:70:PRO:HA	3:E:393:HOH:O	1.98	0.64
1:D:13:VAL:HG21	1:D:19:LEU:CD2	2.28	0.63
1:A:21:LEU:HD12	1:A:75:LEU:HD23	1.82	0.62
2:E:34:TRP:CH2	3:E:474:HOH:O	2.51	0.62
2:B:197:ALA:O	2:B:201:GLN:HG3	2.00	0.62
2:E:15:ARG:HE	2:E:84:GLN:HE21	1.48	0.62
1:D:34:GLN:HE22	2:E:102:LEU:H	1.48	0.62
2:B:7:ASN:HB2	3:B:346:HOH:O	2.00	0.61
1:A:49:LEU:HD12	2:B:101:GLU:HG3	1.82	0.61
1:D:18:ASN:ND2	1:D:79:ALA:H	1.98	0.60
1:D:109:LEU:HD22	1:D:111:ARG:NH2	2.18	0.58
2:E:62:SER:HA	3:E:449:HOH:O	2.02	0.58
2:E:15:ARG:HE	2:E:84:GLN:HG3	1.72	0.55
2:B:21:PHE:HZ	2:B:110:LEU:HB2	1.72	0.54
1:D:173:SER:OG	2:E:192:ARG:HD2	2.07	0.54
1:A:48:LEU:HD21	1:A:59:SER:HB3	1.90	0.54
2:E:50:GLN:HB3	3:E:473:HOH:O	2.08	0.54
2:B:129:PRO:HD3	2:B:142:LEU:HG	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:217:SER:OG	2:E:218:GLU:N	2.41	0.53
2:E:78:GLU:HG3	3:E:483:HOH:O	2.09	0.52
1:D:202:SER:HA	1:A:166:SER:O	2.10	0.52
2:E:145:LEU:HD13	3:E:365:HOH:O	2.11	0.51
1:A:74:THR:HG22	3:A:326:HOH:O	2.10	0.51
1:D:158:ASP:HB2	3:D:338:HOH:O	2.11	0.51
2:E:143:VAL:HG22	2:E:192:ARG:HG3	1.92	0.50
2:E:53:ALA:HB3	3:E:473:HOH:O	2.11	0.50
1:D:190:ASN:ND2	3:D:374:HOH:O	2.45	0.50
1:D:204:GLU:CD	1:D:204:GLU:H	2.15	0.50
1:A:18:ASN:ND2	1:A:79:ALA:H	2.10	0.50
2:E:15:ARG:NE	2:E:84:GLN:HE21	2.10	0.49
1:A:61:ARG:NH2	1:A:84:ASP:OD1	2.29	0.48
1:A:133:SER:HB3	3:A:340:HOH:O	2.12	0.48
1:D:109:LEU:CD2	1:D:111:ARG:NH2	2.77	0.48
2:E:216:LEU:HD22	2:E:229:PRO:HG2	1.95	0.47
2:B:203:PRO:HA	2:B:240:GLY:O	2.13	0.47
1:A:128:LYS:HD3	3:A:398:HOH:O	2.14	0.47
1:A:150:LYS:HD2	3:A:422:HOH:O	2.15	0.47
1:A:18:ASN:HD22	1:A:78:ALA:HA	1.80	0.47
1:A:50:ILE:CD1	1:A:57:GLN:HB3	2.45	0.47
1:A:125:ARG:HB3	3:A:424:HOH:O	2.14	0.46
1:D:21:LEU:HD22	1:D:106:THR:HG21	1.97	0.46
2:B:152:ASP:HB2	2:B:175:PRO:HG2	1.97	0.46
2:E:10:HIS:HD2	2:E:153:HIS:ND1	2.14	0.46
2:E:163:LYS:HD2	3:E:317:HOH:O	2.14	0.46
1:A:115:GLN:HG2	3:A:427:HOH:O	2.16	0.46
1:A:196:GLU:HG2	3:A:396:HOH:O	2.15	0.46
2:E:55:LEU:HG	3:E:473:HOH:O	2.16	0.46
2:E:198:THR:HG23	3:E:419:HOH:O	2.15	0.45
2:B:218:GLU:HA	2:B:218:GLU:OE2	2.16	0.45
1:D:61:ARG:NH2	1:D:84:ASP:OD1	2.40	0.45
2:E:83:GLU:HB3	3:E:445:HOH:O	2.16	0.45
2:E:145:LEU:HG	2:E:147:THR:HG23	1.99	0.45
2:B:148:GLY:O	2:B:186:ARG:HD2	2.17	0.44
2:E:36:ARG:HD3	2:E:46:LEU:HD21	1.98	0.44
2:E:206:HIS:HE1	2:E:237:GLU:OE2	2.01	0.43
2:B:176:LEU:HD12	2:B:188:ALA:HB3	2.00	0.43
2:B:83:GLU:HB2	3:B:378:HOH:O	2.17	0.43
2:E:153:HIS:HB3	2:E:214:TYR:HB2	1.99	0.43
1:D:13:VAL:HG11	1:D:19:LEU:HD22	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:18:ASN:HD22	1:A:79:ALA:H	1.67	0.43
2:E:116:LEU:HD22	2:E:216:LEU:HD11	2.01	0.43
1:A:49:LEU:HD23	1:A:50:ILE:N	2.34	0.42
2:B:129:PRO:HD2	2:B:200:TRP:CZ2	2.55	0.42
2:B:176:LEU:CD1	2:B:188:ALA:HB3	2.49	0.42
2:B:155:GLU:HG3	2:B:214:TYR:HE1	1.84	0.42
2:B:7:ASN:CB	3:B:346:HOH:O	2.64	0.42
2:E:9:ARG:NH1	3:E:364:HOH:O	2.49	0.41
1:D:81:GLN:HG2	3:D:373:HOH:O	2.19	0.41
2:E:208:ARG:HD2	3:E:323:HOH:O	2.20	0.41
2:E:52:GLU:CD	2:E:52:GLU:H	2.25	0.40
2:B:31:ARG:HD2	3:B:432:HOH:O	2.21	0.40
1:D:58:THR:HG22	1:D:63:ASN:HD22	1.85	0.40
1:A:63:ASN:C	1:A:63:ASN:HD22	2.25	0.40
2:E:145:LEU:HB2	3:E:365:HOH:O	2.20	0.40
1:D:2:GLN:HB3	1:D:101:ILE:HD13	2.03	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	202/205 (98%)	196 (97%)	6 (3%)	0	100	100
1	D	202/205 (98%)	196 (97%)	6 (3%)	0	100	100
2	B	240/244 (98%)	234 (98%)	6 (2%)	0	100	100
2	E	240/244 (98%)	233 (97%)	7 (3%)	0	100	100
All	All	884/898 (98%)	859 (97%)	25 (3%)	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	182/183 (100%)	175 (96%)	7 (4%)	33	31
1	D	182/183 (100%)	174 (96%)	8 (4%)	28	25
2	B	213/215 (99%)	201 (94%)	12 (6%)	21	17
2	E	213/215 (99%)	199 (93%)	14 (7%)	16	12
All	All	790/796 (99%)	749 (95%)	41 (5%)	23	19

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	19	LEU
1	D	42	LYS
1	D	58	THR
1	D	68	LYS
1	D	109	LEU
1	D	111	ARG
1	D	148	GLN
1	D	180	LYS
2	E	13	THR
2	E	24	ASP
2	E	27	SER
2	E	39	LEU
2	E	58	SER
2	E	109	ARG
2	E	179	GLN
2	E	182	LEU
2	E	183	ASN
2	E	192	ARG
2	E	208	ARG
2	E	212	GLN
2	E	216	LEU
2	E	243	ASP
1	A	42	LYS
1	A	63	ASN

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Mol	Chain	Res	Type
1	A	74	THR
1	A	95	ASP
1	A	128	LYS
1	A	151	ASP
1	A	204	GLU
2	B	13	THR
2	B	39	LEU
2	B	50	GLN
2	B	59	ARG
2	B	84	GLN
2	B	109	ARG
2	B	176	LEU
2	B	179	GLN
2	B	192	ARG
2	B	204	ARG
2	B	217	SER
2	B	225	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	18	ASN
1	D	34	GLN
1	D	63	ASN
1	D	190	ASN
2	E	10	HIS
2	E	30	ASN
2	E	41	GLN
2	E	51	ASN
2	E	84	GLN
2	E	118	ASN
2	E	179	GLN
2	E	183	ASN
2	E	206	HIS
1	A	18	ASN
1	A	63	ASN
1	A	115	GLN
1	A	143	GLN
1	A	179	ASN
1	A	190	ASN
2	B	80	GLN
2	B	179	GLN

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Mol	Chain	Res	Type
2	B	183	ASN

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 [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	204/205 (99%)	0.75	21 (10%) 6 6	13, 25, 48, 65	0
1	D	204/205 (99%)	0.33	7 (3%) 45 44	10, 20, 36, 57	0
2	B	242/244 (99%)	0.41	9 (3%) 41 41	12, 25, 41, 61	0
2	E	242/244 (99%)	0.67	19 (7%) 12 11	11, 25, 40, 55	0
All	All	892/898 (99%)	0.54	56 (6%) 20 19	10, 24, 41, 65	0

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	167	MET	8.7
1	D	204	GLU	6.2
2	E	2	THR	5.9
2	B	218	GLU	5.6
1	A	40	PRO	5.6
1	A	129	SER	5.3
1	A	169	PHE	5.3
1	A	166	SER	5.0
1	A	162	LEU	4.9
1	A	165	ARG	4.9
2	E	243	ASP	4.8
1	A	168	ASP	4.7
2	E	59	ARG	4.5
1	A	181	SER	4.4
1	A	131	ASP	4.4
2	E	183	ASN	4.4
1	D	96	SER	4.3
1	A	204	GLU	4.2
2	B	2	THR	4.0
1	D	203	PRO	3.9
1	A	150	LYS	3.7

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Mol	Chain	Res	Type	RSRZ
2	B	243	ASP	3.6
2	E	218	GLU	3.5
1	D	41	GLY	3.4
2	B	242	ALA	3.4
1	A	163	ASP	3.3
2	B	241	ARG	3.2
2	B	97	TRP	3.1
2	B	223	THR	3.0
1	A	151	ASP	3.0
1	A	130	SER	3.0
1	A	41	GLY	3.0
2	E	181	ALA	2.9
2	E	28	GLU	2.9
2	E	242	ALA	2.8
2	E	180	PRO	2.8
2	E	184	ASP	2.8
1	D	182	ASP	2.7
2	E	241	ARG	2.7
2	E	16	GLY	2.7
1	D	40	PRO	2.5
2	B	39	LEU	2.5
2	E	27	SER	2.5
1	D	168	ASP	2.4
2	E	179	GLN	2.4
1	A	90	CYS	2.3
2	E	39	LEU	2.3
1	A	96	SER	2.3
1	A	1	LYS	2.2
1	A	152	SER	2.2
1	A	115	GLN	2.2
2	E	182	LEU	2.1
2	E	225	ASP	2.1
2	B	9	ARG	2.1
2	E	13	THR	2.0
2	E	74	PHE	2.0

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.