



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 4, 2023 – 04:55 PM EDT

PDB ID : 4PRH
Title : Crystal structure of TK3 TCR-HLA-B*35:08-HPVG-D5 complex
Authors : Yu Chih, L.; Rossjohn, J.; Gras, S.
Deposited on : 2014-03-05
Resolution : 2.50 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 : 2.35.1
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) : 2.35.1

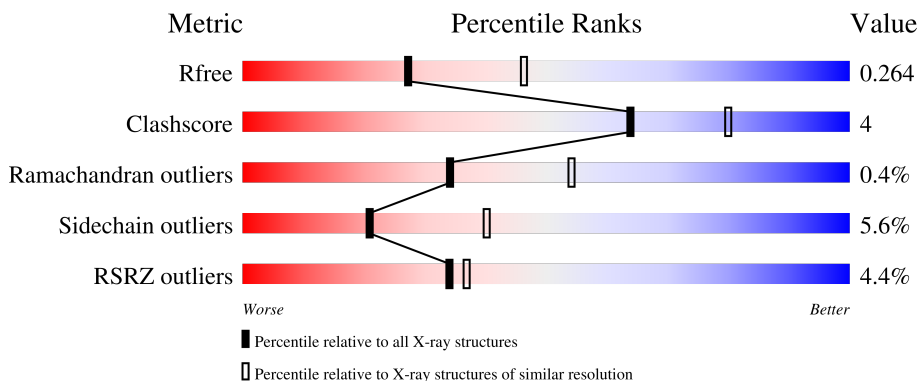
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	272	 4% 76% 11% 12%
2	B	100	 22% 65% 18% 14%
3	C	11	 82% 18%
4	D	208	 % 86% 11% %
5	E	243	 84% 13% % %

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 6346 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 MHC class I antigen.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	240	1975	1236	362	370	7	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	GLN	deletion	UNP C5MK56
A	?	-	THR	deletion	UNP C5MK56

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	86	717	460	121	134	2	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	MET	-	expression tag	UNP P61769
B	1	ILE	-	expression tag	UNP P61769
B	2	GLN	-	expression tag	UNP P61769
B	46	LEU	ILE	conflict	UNP P61769

- Molecule 3 is a protein called Epstein-Barr nuclear antigen 1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	C	11	94	61	13	20	0	0	0

- Molecule 4 is a protein called TK3 TCR alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	202	1583	985	261	330	7	0	1	0

- Molecule 5 is a protein called TK3 TCR beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	E	240	1911	1203	333	370	5	0	0	0

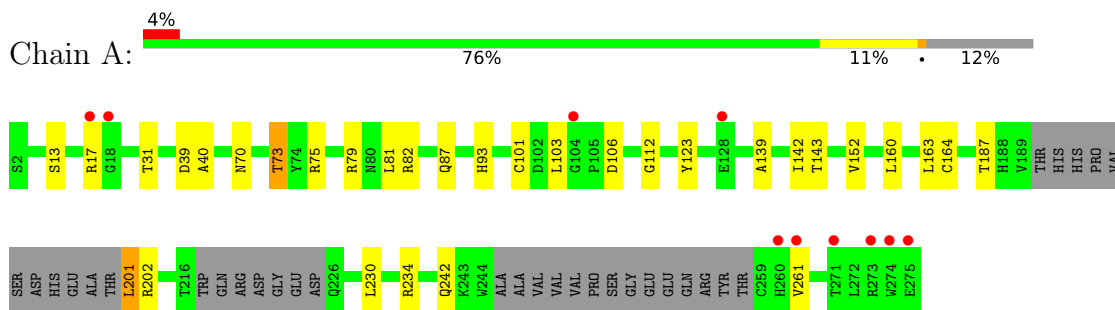
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	11	Total	O	0	0
			11	11		
6	C	3	Total	O	0	0
			3	3		
6	D	26	Total	O	0	0
			26	26		
6	E	26	Total	O	0	0
			26	26		

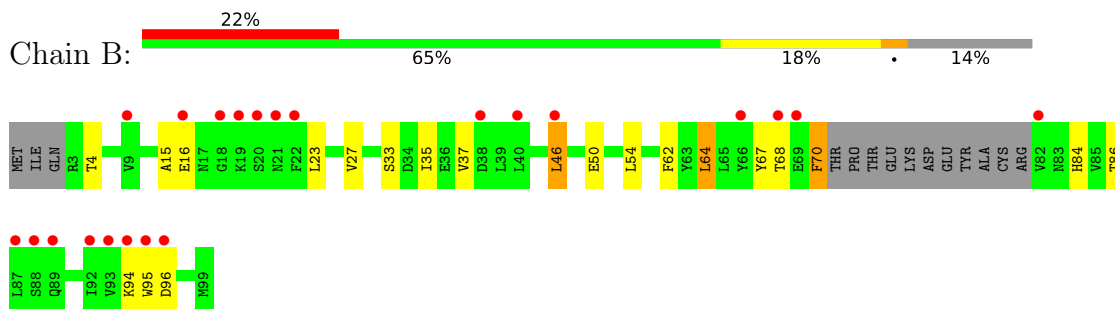
3 Residue-property plots [i](#)

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.

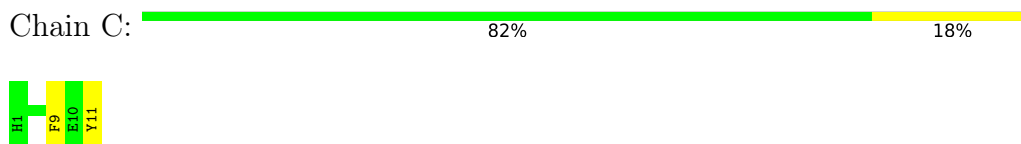
- Molecule 1: MHC class I antigen



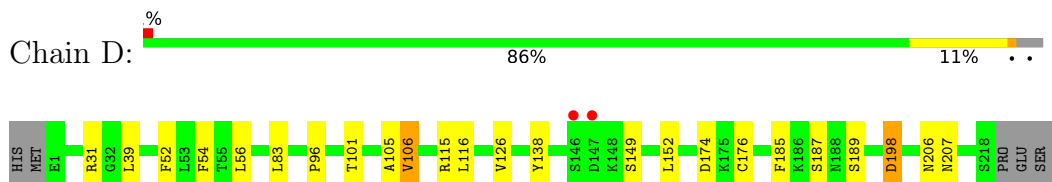
- Molecule 2: Beta-2-microglobulin



- Molecule 3: Epstein-Barr nuclear antigen 1



- Molecule 4: TK3 TCR alpha chain



- Molecule 5: TK3 TCR beta chain

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	44.84Å 62.08Å 98.33Å 92.70° 101.92° 108.21°	Depositor
Resolution (Å)	35.68 – 2.50 35.68 – 2.50	Depositor EDS
% Data completeness (in resolution range)	97.0 (35.68-2.50) 97.0 (35.68-2.50)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.08 (at 2.51Å)	Xtrriage
Refinement program	PHENIX, BUSTER 2.10.0	Depositor
R, R_{free}	0.212 , 0.253 0.218 , 0.264	Depositor DCC
R_{free} test set	1635 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	49.2	Xtrriage
Anisotropy	0.432	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 45.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6346	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.23% 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	0.46	0/2026	0.72	0/2745
2	B	0.45	0/737	0.76	0/997
3	C	0.59	0/98	0.66	0/132
4	D	0.49	0/1615	0.75	0/2187
5	E	0.47	0/1960	0.75	1/2664 (0.0%)
All	All	0.47	0/6436	0.74	1/8725 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	162	PRO	C-N-CA	5.11	134.47	121.70

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	1975	0	1872	13	0
2	B	717	0	680	10	0
3	C	94	0	74	2	0
4	D	1583	0	1508	9	0
5	E	1911	0	1818	18	0
6	A	11	0	0	0	0
6	C	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	D	26	0	0	0	0
6	E	26	0	0	0	0
All	All	6346	0	5952	47	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 4.

All (47) 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)
4:D:176:CYS:HG	5:E:181:CYS:HG	0.86	0.81
1:A:13:SER:HB2	1:A:93:HIS:H	1.51	0.75
1:A:101:CYS:HG	1:A:164:CYS:HG	1.35	0.73
2:B:33:SER:HB2	2:B:54:LEU:HD21	1.71	0.73
2:B:94:LYS:HG3	2:B:95:TRP:H	1.60	0.66
5:E:84:ASP:OD2	5:E:86:HIS:HD2	1.79	0.65
2:B:84:HIS:ND1	2:B:86:THR:HG22	2.16	0.60
1:A:70:ASN:HA	1:A:73:THR:HG23	1.83	0.59
1:A:201:LEU:HB2	1:A:202:ARG:HA	1.84	0.58
2:B:4:THR:HA	2:B:86:THR:HG21	1.85	0.57
2:B:95:TRP:HB3	2:B:96:ASP:HB2	1.86	0.56
1:A:75:ARG:HH21	1:A:79:ARG:HH21	1.54	0.55
2:B:27:VAL:HG11	2:B:37:VAL:HG21	1.87	0.55
5:E:167:LEU:HD21	5:E:220:CYS:SG	2.48	0.54
4:D:39:LEU:HD23	4:D:106:VAL:HG23	1.90	0.54
1:A:82:ARG:HB2	1:A:87:GLN:HB2	1.90	0.53
1:A:139:ALA:HA	1:A:142:ILE:HD12	1.92	0.52
5:E:212:GLN:HA	5:E:252:ARG:O	2.10	0.52
5:E:21:LEU:HD12	5:E:89:LEU:HD23	1.94	0.50
5:E:84:ASP:OD2	5:E:86:HIS:CD2	2.62	0.50
5:E:44:GLN:HB2	5:E:50:LEU:HD13	1.95	0.49
5:E:122:THR:OG1	5:E:164:HIS:HE1	1.96	0.48
4:D:39:LEU:CD2	4:D:106:VAL:HG23	2.44	0.48
4:D:105:ALA:HB1	4:D:116:LEU:HB3	1.94	0.48
4:D:138:TYR:CE2	5:E:144:GLU:HG3	2.49	0.47
1:A:81:LEU:HD21	1:A:123:TYR:CZ	2.49	0.47
1:A:234:ARG:HE	1:A:242:GLN:HE21	1.62	0.47
5:E:39:VAL:HG11	5:E:87:SER:CB	2.44	0.47
1:A:187:THR:HG21	1:A:261:VAL:HG21	1.96	0.46
5:E:155:CYS:CB	5:E:220:CYS:HG	2.24	0.46
2:B:46:LEU:HD22	2:B:68:THR:HG21	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:54:LEU:HD11	2:B:62:PHE:HB3	1.98	0.46
5:E:19:VAL:HG22	5:E:94:LEU:HD11	1.99	0.45
5:E:140:PRO:HD3	5:E:153:LEU:HG	1.98	0.45
4:D:52:PHE:CZ	5:E:112:GLU:HG2	2.52	0.44
5:E:14:ALA:HA	5:E:124:LEU:O	2.18	0.44
2:B:54:LEU:HD13	2:B:64:LEU:HD23	2.01	0.43
4:D:96:PRO:HA	4:D:126:VAL:HB	2.01	0.42
4:D:56:LEU:HD13	4:D:83:LEU:HB2	2.01	0.42
1:A:112:GLY:HA3	1:A:160:LEU:HD13	2.03	0.41
4:D:185:PHE:CE2	4:D:187:SER:HB2	2.55	0.41
5:E:18:ARG:HG3	5:E:92:SER:HB3	2.03	0.41
5:E:181:CYS:HB3	5:E:203:ARG:HD2	2.03	0.41
1:A:152:VAL:HG22	3:C:9:PHE:CE2	2.56	0.41
5:E:26:ARG:HB3	5:E:29:ASP:OD2	2.21	0.41
2:B:23:LEU:HB2	2:B:70:PHE:CE2	2.55	0.40
1:A:143:THR:HG23	3:C:11:TYR:HA	2.03	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	232/272 (85%)	218 (94%)	13 (6%)	1 (0%)	34	54
2	B	82/100 (82%)	70 (85%)	11 (13%)	1 (1%)	13	24
3	C	9/11 (82%)	8 (89%)	1 (11%)	0	100	100
4	D	201/208 (97%)	192 (96%)	8 (4%)	1 (0%)	29	48
5	E	238/243 (98%)	230 (97%)	8 (3%)	0	100	100
All	All	762/834 (91%)	718 (94%)	41 (5%)	3 (0%)	34	54

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	15	ALA
1	A	40	ALA
4	D	198	ASP

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	204/231 (88%)	195 (96%)	9 (4%)	28	52
2	B	81/95 (85%)	74 (91%)	7 (9%)	10	20
3	C	9/9 (100%)	9 (100%)	0	100	100
4	D	181/186 (97%)	169 (93%)	12 (7%)	16	32
5	E	208/211 (99%)	198 (95%)	10 (5%)	25	48
All	All	683/732 (93%)	645 (94%)	38 (6%)	21	40

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	ARG
1	A	31	THR
1	A	39	ASP
1	A	73	THR
1	A	103	LEU
1	A	106	ASP
1	A	163	LEU
1	A	201	LEU
1	A	230	LEU
2	B	16	GLU
2	B	35	ILE
2	B	46	LEU
2	B	50	GLU
2	B	64	LEU
2	B	67	TYR
2	B	70	PHE
4	D	31	ARG

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Mol	Chain	Res	Type
4	D	54	PHE
4	D	101	THR
4	D	106	VAL
4	D	115	ARG
4	D	149	SER
4	D	152	LEU
4	D	174	ASP
4	D	189	SER
4	D	198	ASP
4	D	206	ASN
4	D	207	ASN
5	E	13	THR
5	E	24	SER
5	E	31	SER
5	E	70	ASN
5	E	84	ASP
5	E	112	GLU
5	E	181	CYS
5	E	203	ARG
5	E	235	GLN
5	E	236	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	127	ASN
1	A	141	GLN
1	A	242	GLN
4	D	159	GLN
5	E	70	ASN
5	E	86	HIS
5	E	164	HIS
5	E	212	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	240/272 (88%)	0.14	10 (4%) 36 39	42, 66, 97, 140	61 (25%)
2	B	86/100 (86%)	1.16	22 (25%) 0 0	51, 85, 110, 120	40 (46%)
3	C	11/11 (100%)	-0.61	0 100 100	38, 43, 52, 60	0
4	D	202/208 (97%)	-0.32	2 (0%) 82 84	24, 47, 79, 96	29 (14%)
5	E	240/243 (98%)	-0.38	0 100 100	25, 47, 76, 96	18 (7%)
All	All	779/834 (93%)	-0.04	34 (4%) 34 37	24, 55, 97, 140	148 (18%)

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	18	GLY	9.3
2	B	18	GLY	8.0
2	B	95	TRP	7.1
1	A	275	GLU	6.5
1	A	274	TRP	6.3
1	A	17	ARG	5.5
4	D	146	SER	5.5
1	A	273	ARG	5.3
2	B	93	VAL	4.9
2	B	87	LEU	4.7
2	B	92	ILE	4.7
2	B	20	SER	4.3
2	B	94	LYS	4.3
4	D	147	ASP	4.3
2	B	21	ASN	4.2
2	B	19	LYS	3.6
2	B	38	ASP	3.4
2	B	96	ASP	3.1
2	B	40	LEU	2.5
2	B	69	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
2	B	16	GLU	2.4
1	A	104	GLY	2.3
1	A	260	HIS	2.3
2	B	9	VAL	2.3
2	B	22	PHE	2.2
2	B	88	SER	2.2
1	A	261	VAL	2.2
1	A	271	THR	2.2
2	B	46	LEU	2.2
2	B	68	THR	2.1
2	B	82	VAL	2.1
2	B	66	TYR	2.1
2	B	89	GLN	2.1
1	A	128	GLU	2.1

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.