



Full wwPDB X-ray Structure Validation Report ⓘ

May 20, 2025 – 12:41 PM EDT

PDB ID : 8VTE / pdb_00008vte
Title : Co-structure of the Fab of the anti-TIGIT Vibostolimab antibody with its antigen
Authors : Fischmann, T.; Bahmanjah, S.
Deposited on : 2024-01-26
Resolution : 2.29 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:

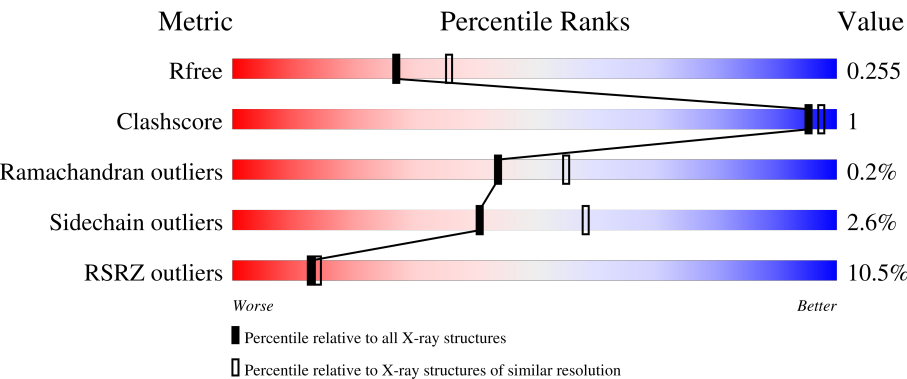
MolProbity : 4-5-2 with Phenix2.0rc1
Xtriage (Phenix) : 2.0rc1
EDS : 3.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.006 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.43.1

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 2.29 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}	164625	5963 (2.30-2.30)
Clashscore	180529	6698 (2.30-2.30)
Ramachandran outliers	177936	6640 (2.30-2.30)
Sidechain outliers	177891	6640 (2.30-2.30)
RSRZ outliers	164620	5963 (2.30-2.30)

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	220	<div><div>3%</div><div>97%</div><div></div></div>
1	C	220	<div><div>14%</div><div>94%</div><div>5%</div></div>
2	B	230	<div><div>4%</div><div>96%</div><div></div></div>
2	D	230	<div><div>8%</div><div>93%</div><div>6%</div></div>
3	E	122	<div><div>34%</div><div>75%</div><div>7%</div><div>19%</div></div>

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Mol	Chain	Length	Quality of chain
3	F	122	<div> <div></div> <div>7%</div> <div>82%</div> <div>6%</div> <div>12%</div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 17016 atoms, of which 8170 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 Tiragolumab antibody light chain variable domains.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	220	Total	C	H	N	O	S	1646	0	0
			3352	1071	1646	282	347	6			
1	C	218	Total	C	H	N	O	S	1635	0	0
			3325	1063	1635	280	342	5			

- Molecule 2 is a protein called Tiragolumab antibody heavy chain variable domains.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	227	Total	C	H	N	O	S	1689	3	0
			3416	1093	1689	286	344	4			
2	D	227	Total	C	H	N	O	S	1681	0	0
			3400	1089	1681	284	342	4			

- Molecule 3 is a protein called T-cell immunoreceptor with Ig and ITIM domains.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	E	99	Total	C	H	N	O	S	728	0	0
			1488	481	728	126	150	3			
3	F	107	Total	C	H	N	O	S	791	0	0
			1610	516	791	134	164	5			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	138	HIS	-	expression tag	UNP Q495A1
E	139	HIS	-	expression tag	UNP Q495A1
E	140	HIS	-	expression tag	UNP Q495A1
E	141	HIS	-	expression tag	UNP Q495A1
E	142	HIS	-	expression tag	UNP Q495A1
E	143	HIS	-	expression tag	UNP Q495A1
F	138	HIS	-	expression tag	UNP Q495A1
F	139	HIS	-	expression tag	UNP Q495A1

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Chain	Residue	Modelled	Actual	Comment	Reference
F	140	HIS	-	expression tag	UNP Q495A1
F	141	HIS	-	expression tag	UNP Q495A1
F	142	HIS	-	expression tag	UNP Q495A1
F	143	HIS	-	expression tag	UNP Q495A1

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	120	Total 120	O 120	0	0
4	B	109	Total 109	O 109	0	0
4	C	51	Total 51	O 51	0	0
4	D	103	Total 103	O 103	0	0
4	E	8	Total 8	O 8	0	0
4	F	34	Total 34	O 34	0	0

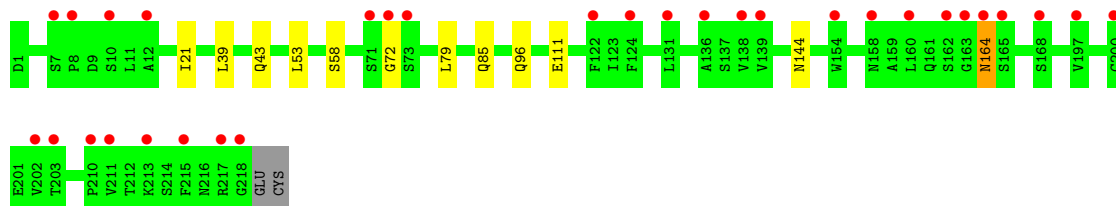
3 Residue-property plots [i](#)

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.

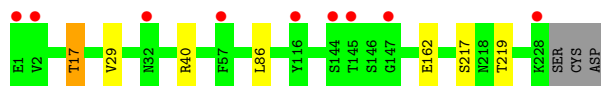
- Molecule 1: Tiragolumab antibody light chain variable domains



- Molecule 1: Tiragolumab antibody light chain variable domains



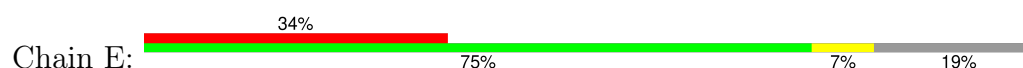
- Molecule 2: Tiragolumab antibody heavy chain variable domains

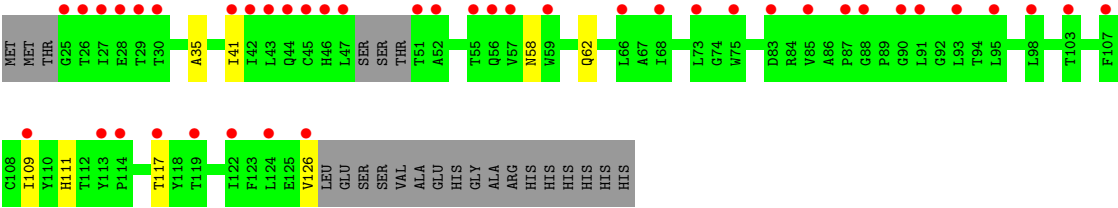


- Molecule 2: Tiragolumab antibody heavy chain variable domains

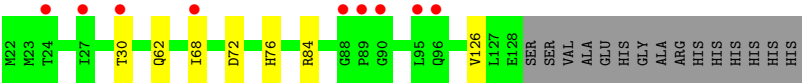
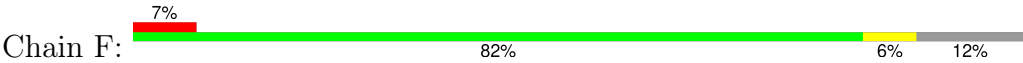


- Molecule 3: T-cell immunoreceptor with Ig and ITIM domains





● Molecule 3: T-cell immunoreceptor with Ig and ITIM domains



4 Data and refinement statistics

Property	Value	Source
Space group	I 4	Depositor
Cell constants a, b, c, α , β , γ	213.69Å 213.69Å 66.43Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.21 – 2.29 33.21 – 2.29	Depositor EDS
% Data completeness (in resolution range)	73.5 (33.21-2.29) 73.4 (33.21-2.29)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.90 (at 2.29Å)	Xtriage
Refinement program	BUSTER 2.11.8	Depositor
R, R_{free}	0.229 , 0.268 0.219 , 0.255	Depositor DCC
R_{free} test set	20482 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	46.3	Xtriage
Anisotropy	0.009	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 49.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.010 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	17016	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.07% 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	0.72	0/1745	0.93	0/2372
1	C	0.70	0/1729	0.91	1/2352 (0.0%)
2	B	0.71	0/1786	0.90	0/2442
2	D	0.72	1/1764 (0.1%)	0.88	0/2412
3	E	0.74	0/776	0.92	0/1058
3	F	0.78	1/836 (0.1%)	0.97	0/1140
All	All	0.72	2/8636 (0.0%)	0.91	1/11776 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	89	VAL	CA-CB	5.28	1.60	1.54
3	F	62	GLN	CA-C	5.02	1.57	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	164	ASN	CA-CB-CG	6.77	119.37	112.60

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	1706	1646	1649	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1690	1635	1638	4	0
2	B	1727	1689	1674	2	0
2	D	1719	1681	1684	8	0
3	E	760	728	728	3	0
3	F	819	791	788	1	0
4	A	120	0	0	2	0
4	B	109	0	0	2	0
4	C	51	0	0	2	0
4	D	103	0	0	3	0
4	E	8	0	0	0	0
4	F	34	0	0	0	0
All	All	8846	8170	8161	19	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 1.

All (19) 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:B:348:HOH:O	2:D:13:LYS:HE3	1.86	0.74
2:D:1:GLU:HA	4:D:328:HOH:O	1.89	0.72
1:C:72:GLY:HA2	4:C:343:HOH:O	1.92	0.68
2:B:17:THR:HG22	4:B:329:HOH:O	1.94	0.67
2:D:35:ALA:HB3	2:D:102:GLU:HB3	1.84	0.58
1:C:43:GLN:HB2	1:C:53:LEU:HD11	1.90	0.53
3:E:111:HIS:CD2	3:E:117:THR:HG22	2.43	0.52
3:E:35:ALA:HB2	3:E:41:ILE:HD13	1.92	0.51
1:A:87:GLU:HG2	4:A:380:HOH:O	2.12	0.49
1:C:21:ILE:HD11	1:C:79:LEU:HD23	1.94	0.47
1:C:111:GLU:HG2	4:C:316:HOH:O	2.14	0.47
3:E:109:ILE:CG2	3:E:111:HIS:CE1	3.00	0.44
2:D:100:THR:OG1	2:D:114:PHE:HB3	2.18	0.43
2:D:45:ARG:HD3	4:D:354:HOH:O	2.18	0.42
2:D:108:LEU:HD12	3:F:76:HIS:CD2	2.54	0.42
2:B:217:SER:HG	2:B:219:THR:HG1	1.54	0.41
1:A:37:LYS:HE3	4:A:315:HOH:O	2.20	0.41
2:D:150:ALA:HA	4:D:358:HOH:O	2.21	0.41
2:D:14:PRO:O	2:D:15:SER:OG	2.34	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	218/220 (99%)	213 (98%)	5 (2%)	0	100	100
1	C	216/220 (98%)	208 (96%)	7 (3%)	1 (0%)	25	32
2	B	228/230 (99%)	222 (97%)	6 (3%)	0	100	100
2	D	225/230 (98%)	218 (97%)	7 (3%)	0	100	100
3	E	95/122 (78%)	92 (97%)	2 (2%)	1 (1%)	12	13
3	F	105/122 (86%)	99 (94%)	6 (6%)	0	100	100
All	All	1087/1144 (95%)	1052 (97%)	33 (3%)	2 (0%)	44	55

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	144	ASN
3	E	62	GLN

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	195/195 (100%)	190 (97%)	5 (3%)	41	58
1	C	193/195 (99%)	188 (97%)	5 (3%)	41	58
2	B	201/201 (100%)	196 (98%)	5 (2%)	42	60
2	D	198/201 (98%)	195 (98%)	3 (2%)	60	76
3	E	83/103 (81%)	81 (98%)	2 (2%)	44	61

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	F	91/103 (88%)	86 (94%)	5 (6%)	18	26
All	All	961/998 (96%)	936 (97%)	25 (3%)	41	58

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	SER
1	A	39	LEU
1	A	54	ILE
1	A	64	VAL
1	A	219	GLU
2	B	17	THR
2	B	29	VAL
2	B	40	ARG
2	B	86	LEU
2	B	162	GLU
1	C	39	LEU
1	C	58	SER
1	C	85	GLN
1	C	96	GLN
1	C	164	ASN
2	D	29	VAL
2	D	89	VAL
2	D	219	THR
3	E	58	ASN
3	E	126	VAL
3	F	30	THR
3	F	68	ILE
3	F	72	ASP
3	F	84	ARG
3	F	126	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	ASN
1	A	44	GLN
1	A	195	HIS
2	B	32	ASN
2	B	41	GLN
2	B	213	ASN

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Mol	Chain	Res	Type
1	C	43	GLN
1	C	44	GLN
1	C	161	GLN
1	C	195	HIS
2	D	41	GLN
3	E	64	GLN
3	E	111	HIS
3	F	76	HIS

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 oligosaccharides 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	220/220 (100%)	0.05	6 (2%) 56 57	15, 23, 33, 49	0
1	C	218/220 (99%)	0.90	31 (14%) 7 8	17, 33, 62, 71	0
2	B	227/230 (98%)	0.20	9 (3%) 43 44	14, 23, 34, 45	1 (0%)
2	D	227/230 (98%)	0.45	18 (7%) 20 22	15, 24, 61, 73	0
3	E	99/122 (81%)	1.97	42 (42%) 1 1	25, 50, 74, 87	0
3	F	107/122 (87%)	0.81	9 (8%) 18 20	17, 31, 46, 61	0
All	All	1098/1144 (95%)	0.58	115 (10%) 13 14	14, 27, 61, 87	1 (0%)

All (115) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	147	GLY	6.1
1	C	7	SER	5.8
3	E	47	LEU	5.2
3	E	27	ILE	5.0
3	E	68	ILE	5.0
3	F	24	THR	4.6
1	C	218	GLY	4.5
1	A	7	SER	4.5
2	D	145	THR	4.3
3	E	25	GLY	4.2
2	D	228	LYS	4.1
1	C	160	LEU	4.0
3	E	90	GLY	3.9
2	D	142	SER	3.9
1	C	72	GLY	3.8
3	E	26	THR	3.8
3	E	28	GLU	3.7
2	B	1	GLU	3.7
3	E	42	ILE	3.7

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Mol	Chain	Res	Type	RSRZ
1	C	203	THR	3.7
1	A	220	CYS	3.6
3	E	41	ILE	3.6
3	E	46	HIS	3.6
3	E	126	VAL	3.6
3	E	93	LEU	3.5
3	E	43	LEU	3.5
3	E	113	TYR	3.4
3	E	122	ILE	3.3
2	D	32	ASN	3.3
1	C	163	GLY	3.3
1	C	139	VAL	3.3
3	E	88	GLY	3.3
2	B	145	THR	3.2
1	C	200	CYS	3.2
2	D	143	LYS	3.2
3	E	56	GLN	3.1
3	E	51	THR	3.1
1	C	73	SER	3.1
2	B	147	GLY	3.0
1	C	10	SER	3.0
1	C	138	VAL	3.0
1	C	211	VAL	3.0
3	E	30	THR	2.9
3	E	117	THR	2.9
2	D	151	ALA	2.9
2	D	144	SER	2.9
1	C	215	PHE	2.8
1	C	202	VAL	2.8
1	C	213	LYS	2.8
2	D	152	LEU	2.8
3	E	57	VAL	2.8
3	F	90	GLY	2.8
3	E	55	THR	2.8
3	E	44	GLN	2.7
1	C	158	ASN	2.7
2	D	207	THR	2.7
3	E	59	TRP	2.7
3	E	91	LEU	2.7
2	D	203	LEU	2.6
3	E	75	TRP	2.6
3	F	89	PRO	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	197	VAL	2.6
1	C	131	LEU	2.6
3	E	119	THR	2.6
1	C	165	SER	2.6
3	E	107	PHE	2.6
3	F	88	GLY	2.5
1	A	8	PRO	2.5
2	B	116	TYR	2.5
2	D	146	SER	2.5
3	F	68	ILE	2.4
3	E	52	ALA	2.4
1	C	217	ARG	2.4
3	E	29	THR	2.4
2	B	228	LYS	2.4
3	E	114	PRO	2.4
1	C	168	SER	2.4
2	B	144	SER	2.4
2	D	139	ALA	2.4
3	F	27	ILE	2.3
2	D	148	GLY	2.3
3	F	95	LEU	2.3
1	C	136	ALA	2.3
2	D	136	PHE	2.3
1	C	154	TRP	2.3
1	C	12	ALA	2.3
1	C	124	PHE	2.3
3	E	109	ILE	2.3
3	F	96	GLN	2.3
2	B	32	ASN	2.2
3	E	87	PRO	2.2
1	C	162	SER	2.2
3	E	66	LEU	2.2
1	C	8	PRO	2.2
2	B	2	VAL	2.2
3	E	98	LEU	2.2
2	D	135	VAL	2.2
1	C	71	SER	2.2
2	D	66	SER	2.2
1	C	164	ASN	2.2
1	C	122	PHE	2.2
3	E	124	LEU	2.1
1	A	72	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
3	E	45	CYS	2.1
3	E	73	LEU	2.1
2	D	208	TYR	2.0
3	E	85	VAL	2.0
2	B	57	PHE	2.0
1	A	11	LEU	2.0
3	E	95	LEU	2.0
1	A	219	GLU	2.0
3	E	103	THR	2.0
3	F	30	THR	2.0
3	E	83	ASP	2.0
1	C	210	PRO	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.