



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 01:48 PM UTC

PDB ID : 4EI6 / pdb_00004ei6
Title : Structure of XV19 Valpha1-Vbeta16 Type-II Natural Killer T cell receptor
Authors : Patel, O.; Rossjohn, J.
Deposited on : 2012-04-04
Resolution : 1.60 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 Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

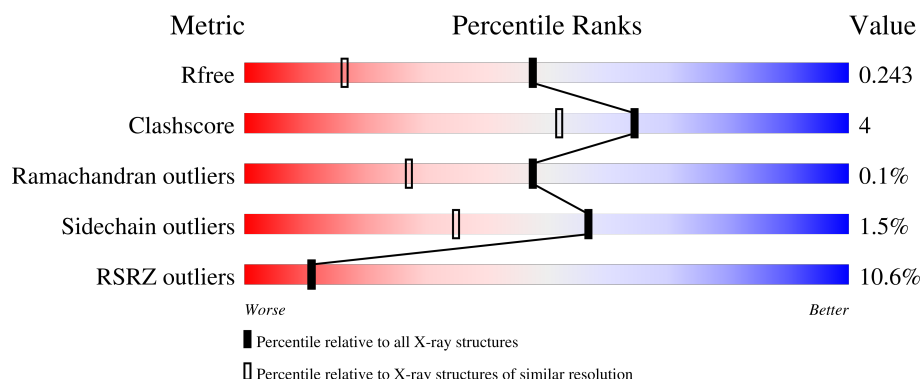
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.60 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}	180053	4673 (1.60-1.60)
Clashscore	190562	4931 (1.60-1.60)
Ramachandran outliers	187476	4831 (1.60-1.60)
Sidechain outliers	187428	4830 (1.60-1.60)
RSRZ outliers	180081	4672 (1.60-1.60)

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 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	208	5% 89% 8% .
1	C	208	14% 84% 6% . 9%
2	B	245	10% 90% 9%
2	D	245	11% 86% 11% ..

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7693 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 Valpha1 XV19 Type II Natural Killer T cell receptor (mouse variable domain, human constant domain).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	202	Total	C	N	O	S	0	11	0
			1573	987	259	317	10			
1	C	189	Total	C	N	O	S	0	8	0
			1469	932	240	288	9			

- Molecule 2 is a protein called Vbeta16 XV19 Type II Natural Killer T cell receptor (mouse variable domain, human constant domain).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	244	Total	C	N	O	S	0	3	0
			1932	1250	321	351	10			
2	D	241	Total	C	N	O	S	0	2	0
			1903	1233	314	347	9			

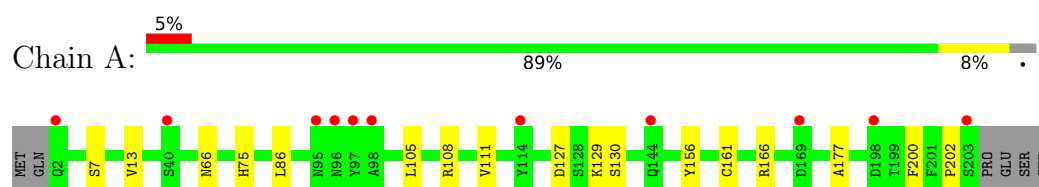
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	231	Total	O	0	0
			231	231		
3	B	240	Total	O	0	0
			240	240		
3	C	173	Total	O	0	0
			173	173		
3	D	172	Total	O	0	0
			172	172		

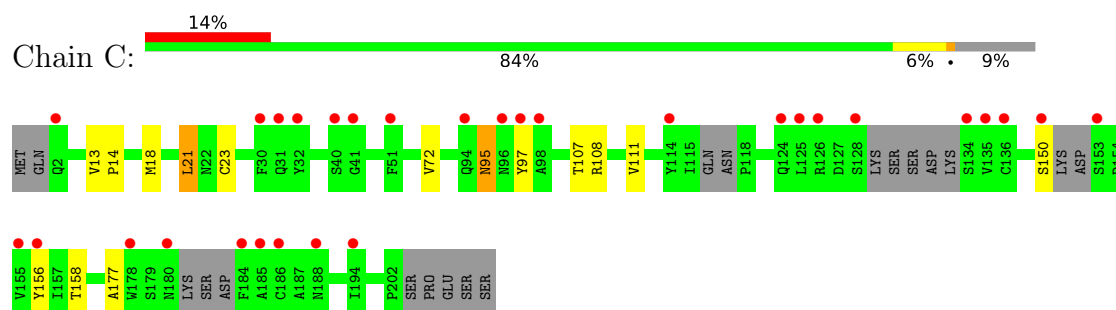
3 Residue-property plots [i](#)

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.

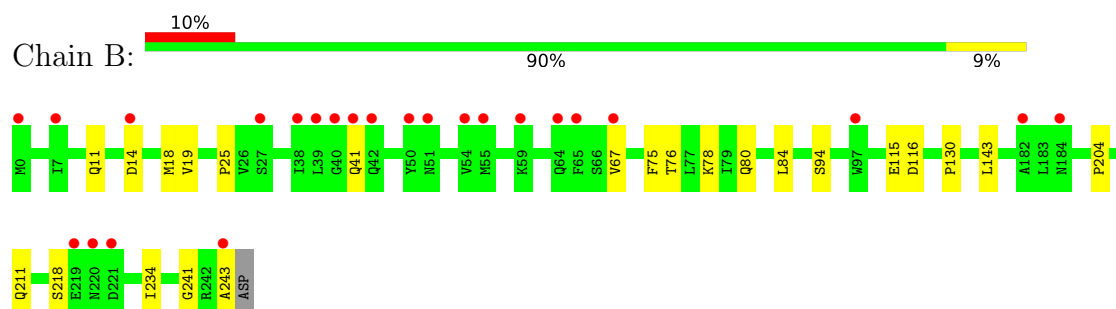
- Molecule 1: Valpha1 XV19 Type II Natural Killer T cell receptor (mouse variable domain, human constant domain)



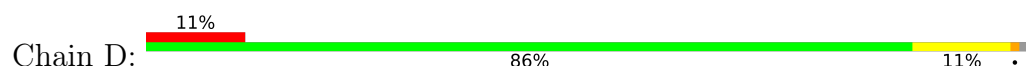
- Molecule 1: Valpha1 XV19 Type II Natural Killer T cell receptor (mouse variable domain, human constant domain)

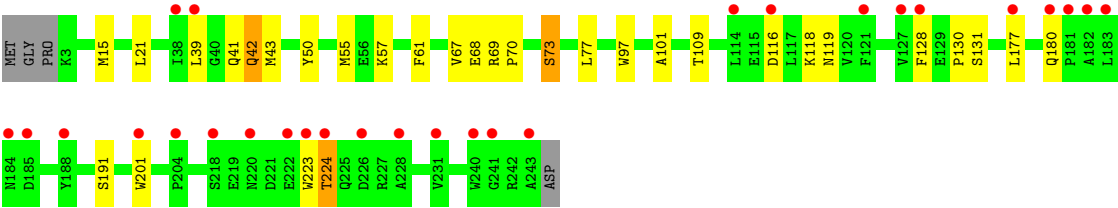


- Molecule 2: Vbeta16 XV19 Type II Natural Killer T cell receptor (mouse variable domain, human constant domain)



- Molecule 2: Vbeta16 XV19 Type II Natural Killer T cell receptor (mouse variable domain, human constant domain)





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	65.27Å 100.12Å 152.67Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.45 – 1.60 44.45 – 1.60	Depositor EDS
% Data completeness (in resolution range)	100.0 (44.45-1.60) 99.9 (44.45-1.60)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.93 (at 1.60Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.4_486)	Depositor
R, R_{free}	0.208 , 0.241 (Not available) , 0.243	Depositor DCC
R_{free} test set	6662 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	21.7	Xtriage
Anisotropy	0.305	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 40.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7693	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.05% 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	0/1645	0.71	0/2236
1	C	0.39	0/1528	0.73	0/2072
2	B	0.41	0/2001	0.71	0/2730
2	D	0.38	0/1970	0.75	2/2694 (0.1%)
All	All	0.40	0/7144	0.72	2/9732 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	180	GLN	CA-C-N	5.14	125.18	119.32
2	D	180	GLN	C-N-CA	5.14	125.18	119.32

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	1573	0	1446	12	0
1	C	1469	0	1355	10	0
2	B	1932	0	1820	13	0
2	D	1903	0	1764	20	0
3	A	231	0	0	2	0
3	B	240	0	0	1	0
3	C	173	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	172	0	0	2	0
All	All	7693	0	6385	51	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 (51) 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)
2:D:42:GLN:HE21	2:D:42:GLN:HA	1.31	0.94
1:A:166:ARG:HG3	1:A:166:ARG:HH11	1.47	0.80
2:D:42:GLN:HE21	2:D:42:GLN:CA	2.03	0.69
2:B:18:MET:HE2	2:B:78:LYS:HE2	1.77	0.65
1:A:129:LYS:HG2	3:A:454:HOH:O	1.97	0.65
2:B:67:VAL:HG23	2:B:76:THR:O	2.02	0.60
2:D:41:GLN:HB3	3:D:387:HOH:O	2.03	0.59
2:D:97[A]:TRP:HB2	2:D:101:ALA:HB2	1.86	0.58
1:C:158:THR:HG21	2:D:191:SER:OG	2.06	0.56
1:A:105:LEU:O	2:B:41:GLN:HG2	2.06	0.55
1:A:75:HIS:HB2	1:C:18:MET:HE1	1.89	0.54
1:A:86[B]:LEU:HG	1:A:108:ARG:NH1	2.23	0.54
2:D:42:GLN:HA	2:D:42:GLN:NE2	2.13	0.52
2:D:42:GLN:NE2	2:D:43:MET:H	2.09	0.51
2:D:116:ASP:HB3	2:D:118:LYS:H	1.75	0.51
2:B:11:GLN:NE2	2:B:19:VAL:HG23	2.26	0.50
2:D:57:LYS:HD2	2:D:61:PHE:CD2	2.47	0.49
1:C:23:CYS:HB3	1:C:72:VAL:HG13	1.96	0.48
2:D:119:ASN:HB2	3:D:373:HOH:O	2.14	0.47
2:D:50:TYR:CZ	2:D:55:MET:HG3	2.49	0.47
1:A:166:ARG:HG3	1:A:166:ARG:NH1	2.18	0.47
2:D:223:TRP:O	2:D:224:THR:HG23	2.16	0.46
1:A:66:ASN:HB2	3:A:352:HOH:O	2.15	0.46
2:B:84:LEU:HD21	2:B:115:GLU:HG3	1.98	0.46
2:B:204:PRO:HD3	2:B:243:ALA:HB2	1.97	0.46
1:C:95:ASN:C	1:C:97:TYR:H	2.22	0.46
2:D:21:LEU:HD22	2:D:109:THR:HG21	1.98	0.46
2:D:21:LEU:HD12	2:D:77:LEU:HD23	1.98	0.45
1:A:7[A]:SER:OG	1:C:14:PRO:HD3	2.17	0.45
2:B:204:PRO:HA	2:B:241:GLY:O	2.17	0.45
2:D:130:PRO:HD2	2:D:201:TRP:CZ2	2.52	0.45
2:D:70:PRO:HB2	2:D:73:SER:OG	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:13:VAL:O	1:C:111:VAL:HA	2.18	0.44
1:A:127:ASP:HB3	1:A:130:SER:O	2.18	0.43
2:B:25:PRO:HB3	2:B:94:SER:HB3	2.00	0.42
2:B:80:GLN:O	2:B:80:GLN:HG3	2.19	0.42
1:C:21[B]:LEU:CD1	1:C:107:THR:HG21	2.49	0.42
2:B:14:ASP:HB2	3:B:490:HOH:O	2.19	0.42
2:B:211:GLN:HG3	2:B:234:ILE:HG23	2.01	0.42
2:D:128:PHE:CD2	2:D:128:PHE:N	2.87	0.42
1:A:13:VAL:O	1:A:111:VAL:HA	2.20	0.42
1:C:108:ARG:NH1	3:C:447:HOH:O	2.52	0.42
2:D:67:VAL:C	2:D:68:GLU:HG3	2.45	0.41
1:A:200:PHE:CE2	1:A:202:PRO:HG3	2.56	0.41
1:C:156:TYR:O	1:C:177:ALA:HA	2.21	0.41
2:B:130:PRO:HD3	2:B:143:LEU:HG	2.02	0.41
2:D:15:MET:HE3	2:D:15:MET:HB2	1.90	0.41
1:A:156:TYR:O	1:A:177:ALA:HA	2.21	0.40
2:B:67:VAL:HG21	2:B:75:PHE:CE1	2.56	0.40
2:D:177:LEU:C	2:D:177:LEU:HD12	2.46	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	211/208 (101%)	208 (99%)	3 (1%)	0	100	100
1	C	187/208 (90%)	184 (98%)	2 (1%)	1 (0%)	24	10
2	B	245/245 (100%)	238 (97%)	7 (3%)	0	100	100
2	D	241/245 (98%)	235 (98%)	6 (2%)	0	100	100
All	All	884/906 (98%)	865 (98%)	18 (2%)	1 (0%)	48	27

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	95	ASN

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	177/185 (96%)	176 (99%)	1 (1%)	78	66
1	C	162/185 (88%)	159 (98%)	3 (2%)	50	27
2	B	203/216 (94%)	201 (99%)	2 (1%)	68	50
2	D	198/216 (92%)	192 (97%)	6 (3%)	36	13
All	All	740/802 (92%)	728 (98%)	12 (2%)	57	33

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	161	CYS
2	B	116	ASP
2	B	218	SER
1	C	21[A]	LEU
1	C	21[B]	LEU
1	C	150	SER
2	D	39	LEU
2	D	42	GLN
2	D	69	ARG
2	D	73	SER
2	D	131	SER
2	D	224	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	80	GLN
1	C	95	ASN
2	D	11	GLN
2	D	42	GLN

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Mol	Chain	Res	Type
2	D	103	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 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	202/208 (97%)	0.27	11 (5%) 31 32	8, 21, 37, 46	12 (5%)
1	C	189/208 (90%)	0.59	30 (15%) 5 4	8, 22, 46, 59	8 (4%)
2	B	244/245 (99%)	0.49	24 (9%) 13 13	11, 23, 41, 50	3 (1%)
2	D	241/245 (98%)	0.83	28 (11%) 9 9	13, 28, 51, 67	2 (0%)
All	All	876/906 (96%)	0.55	93 (10%) 11 11	8, 24, 45, 67	25 (2%)

All (93) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	96	ASN	5.4
1	C	30	PHE	5.2
1	A	97	TYR	5.2
2	D	184	ASN	4.7
1	A	96	ASN	4.7
1	C	97	TYR	4.6
1	C	180	ASN	4.5
2	B	38	ILE	4.0
1	C	153	SER	3.8
2	D	241	GLY	3.5
2	B	220	ASN	3.4
2	B	50	TYR	3.4
1	C	41	GLY	3.4
1	C	98	ALA	3.3
2	B	7	ILE	3.2
2	D	183	LEU	3.2
1	A	114	TYR	3.2
2	D	185	ASP	3.2
2	B	40	GLY	3.2
2	B	243	ALA	3.1
2	D	220	ASN	3.1

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Mol	Chain	Res	Type	RSRZ
2	D	223	TRP	3.0
2	D	204	PRO	3.0
2	B	39	LEU	3.0
1	A	95	ASN	2.9
1	C	51	PHE	2.9
1	C	184	PHE	2.8
2	B	182	ALA	2.8
2	B	219	GLU	2.8
2	D	121	PHE	2.8
2	D	228	ALA	2.8
1	C	125	LEU	2.8
2	D	177	LEU	2.7
1	C	194	ILE	2.7
2	D	182	ALA	2.7
1	C	178	TRP	2.7
2	D	38	ILE	2.7
2	B	64	GLN	2.7
2	D	243	ALA	2.7
1	A	40	SER	2.6
1	A	203	SER	2.6
2	B	97	TRP	2.6
1	C	114	TYR	2.5
2	B	42	GLN	2.5
2	B	67	VAL	2.5
1	C	40	SER	2.4
1	C	94	GLN	2.4
2	B	59	LYS	2.4
1	C	185	ALA	2.4
2	D	188	TYR	2.4
2	D	128	PHE	2.3
2	D	240	TRP	2.3
2	B	54	VAL	2.3
1	C	128	SER	2.3
2	D	226	ASP	2.3
2	D	181	PRO	2.3
1	C	186	CYS	2.3
1	C	135	VAL	2.3
2	B	0	MET	2.3
1	C	134	SER	2.3
1	C	155	VAL	2.3
2	D	180	GLN	2.2
2	B	51	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
2	D	218	SER	2.2
1	A	144	GLN	2.2
1	A	98	ALA	2.2
2	D	114	LEU	2.2
1	C	31	GLN	2.2
1	C	126	ARG	2.2
2	B	184	ASN	2.2
2	B	14	ASP	2.2
2	B	41	GLN	2.2
2	D	222	GLU	2.2
1	C	188	ASN	2.2
2	B	65	PHE	2.2
1	A	169	ASP	2.1
2	D	231	VAL	2.1
2	B	27	SER	2.1
1	C	136	CYS	2.1
1	A	2	GLN	2.1
1	A	198	ASP	2.1
1	C	124	GLN	2.1
1	C	150	SER	2.1
2	B	221	ASP	2.1
2	D	116	ASP	2.1
1	C	32	TYR	2.1
1	C	2	GLN	2.1
2	D	39	LEU	2.1
2	D	224	THR	2.1
2	B	55	MET	2.0
2	D	127	VAL	2.0
2	D	201	TRP	2.0
1	C	156	TYR	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 ⓘ

There are no oligosaccharides 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.