



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 01:54 PM UTC

PDB ID : 2FZ3 / pdb_00002fz3
Title : The role of T cell receptor alpha genes in directing human MHC restriction
Authors : Miles, J.J.; Borg, N.A.
Deposited on : 2006-02-09
Resolution : 1.90 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

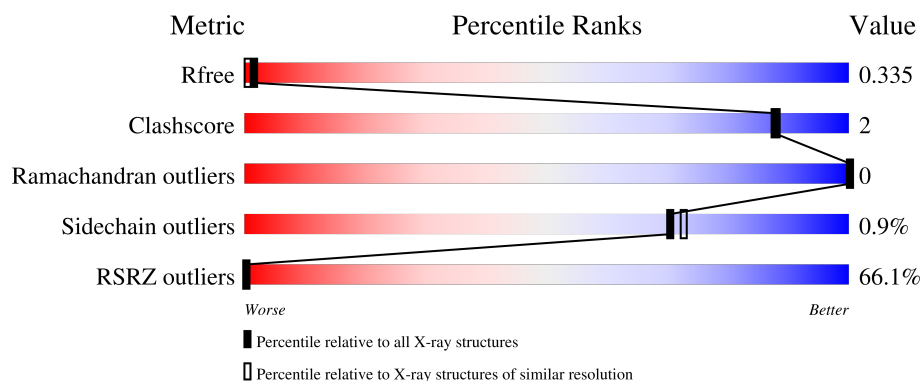
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	276	64% 95% 5%
2	B	99	71% 98% .
3	C	11	73% 100%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 3376 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, B-35 alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	276	Total	C	N	O	S	0	0	0
			2257	1405	414	431	7			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	156	ARG	LEU	SEE REMARK 999	UNP P30474

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	99	Total	C	N	O	S	0	0	0
			829	528	140	158	3			

- Molecule 3 is a protein called 11-mer peptide from Epstein-Barr nuclear antigen 1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	11	Total	C	N	O	0	0	0
			87	56	13	18			

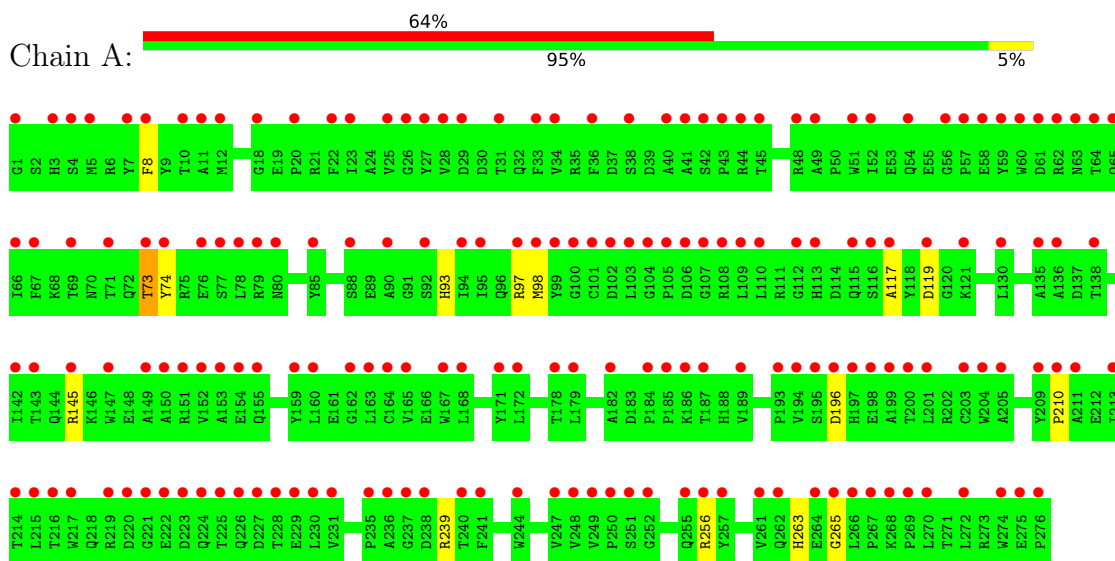
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	153	Total	O	0	0
			153	153		
4	B	42	Total	O	0	0
			42	42		
4	C	8	Total	O	0	0
			8	8		

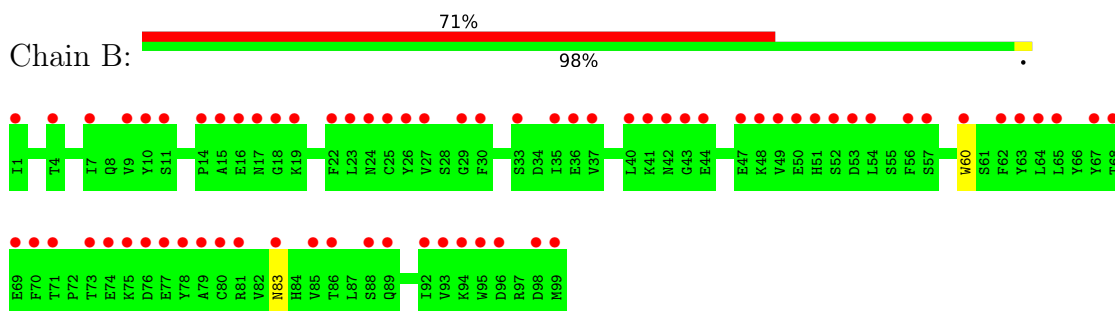
3 Residue-property plots

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.

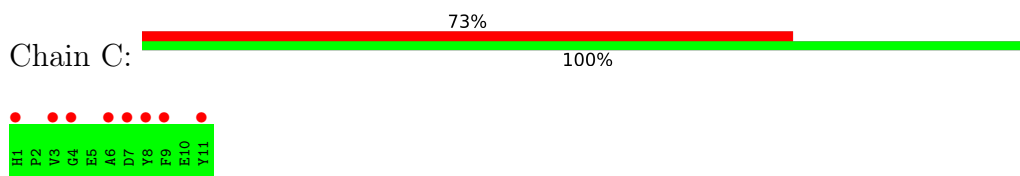
- Molecule 1: HLA class I histocompatibility antigen, B-35 alpha chain



- Molecule 2: Beta-2-microglobulin



- Molecule 3: 11-mer peptide from Epstein-Barr nuclear antigen 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	51.16Å 82.09Å 109.89Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.06 – 1.90 34.06 – 1.90	Depositor EDS
% Data completeness (in resolution range)	98.6 (34.06-1.90) 98.6 (34.06-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.14 (at 1.89Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.232 , 0.275 0.310 , 0.335	Depositor DCC
R_{free} test set	1132 reflections (3.04%)	wwPDB-VP
Wilson B-factor (Å ²)	22.1	Xtriage
Anisotropy	0.466	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 31.8	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	0.89	EDS
Total number of atoms	3376	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.48% 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	0.59	5/2320 (0.2%)	0.76	2/3153 (0.1%)
2	B	0.42	0/852	0.64	0/1152
3	C	0.54	0/90	0.65	0/122
All	All	0.55	5/3262 (0.2%)	0.73	2/4427 (0.0%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	256	ARG	CZ-NH1	6.72	1.42	1.32
1	A	196	ASP	C-O	6.66	1.31	1.24
1	A	256	ARG	CZ-NH2	6.63	1.42	1.33
1	A	256	ARG	CD-NE	5.30	1.53	1.46
1	A	256	ARG	NE-CZ	5.22	1.38	1.33

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	256	ARG	NE-CZ-NH2	-8.33	111.70	119.20
1	A	256	ARG	CD-NE-CZ	-6.21	115.70	124.40

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	2257	0	2119	12	0
2	B	829	0	794	1	0
3	C	87	0	69	0	0
4	A	153	0	0	5	0
4	B	42	0	0	0	0
4	C	8	0	0	0	0
All	All	3376	0	2982	12	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 2.

All (12) 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:93:HIS:HD2	1:A:119:ASP:OD2	1.80	0.65
1:A:263:HIS:CD2	1:A:265:GLY:H	2.17	0.63
1:A:210:PRO:O	1:A:263:HIS:HE1	1.87	0.56
1:A:263:HIS:HD2	1:A:265:GLY:H	1.56	0.54
1:A:93:HIS:HE1	4:A:307:HOH:O	1.90	0.54
1:A:145:ARG:NH1	4:A:312:HOH:O	2.45	0.50
1:A:73:THR:HG22	4:A:385:HOH:O	2.14	0.47
1:A:8:PHE:HE2	1:A:98:MET:HE3	1.81	0.46
1:A:117:ALA:HB2	2:B:60:TRP:CE2	2.54	0.43
1:A:74:TYR:OH	1:A:97:ARG:HD3	2.19	0.42
1:A:73:THR:CG2	4:A:385:HOH:O	2.68	0.42
1:A:145:ARG:HG3	4:A:338:HOH:O	2.21	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	274/276 (99%)	269 (98%)	5 (2%)	0	100	100
2	B	97/99 (98%)	95 (98%)	2 (2%)	0	100	100
3	C	9/11 (82%)	9 (100%)	0	0	100	100
All	All	380/386 (98%)	373 (98%)	7 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	234/234 (100%)	232 (99%)	2 (1%)	70	73
2	B	94/94 (100%)	93 (99%)	1 (1%)	65	67
3	C	8/9 (89%)	8 (100%)	0	100	100
All	All	336/337 (100%)	333 (99%)	3 (1%)	70	73

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	73	THR
1	A	239	ARG
2	B	83	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	70	ASN
1	A	80	ASN
1	A	93	HIS
1	A	224	GLN
1	A	263	HIS
2	B	83	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 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	276/276 (100%)	2.33	177 (64%)  	23, 28, 37, 43	0
2	B	99/99 (100%)	2.53	70 (70%)  	25, 31, 37, 42	0
3	C	11/11 (100%)	2.43	8 (72%)  	23, 30, 35, 37	0
All	All	386/386 (100%)	2.38	255 (66%)  	23, 29, 37, 43	0

All (255) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	197	HIS	5.5
2	B	1	ILE	5.3
1	A	105	PRO	5.1
1	A	103	LEU	5.0
2	B	75	LYS	4.9
1	A	200	THR	4.8
1	A	194	VAL	4.5
2	B	74	GLU	4.5
1	A	193	PRO	4.3
2	B	19	LYS	4.3
3	C	9	PHE	4.2
1	A	149	ALA	4.2
1	A	269	PRO	4.1
1	A	196	ASP	4.0
2	B	69	GLU	4.0
1	A	266	LEU	3.9
2	B	99	MET	3.9
1	A	107	GLY	3.9
2	B	43	GLY	3.9
1	A	67	PHE	3.9
1	A	109	LEU	3.8
1	A	162	GLY	3.7
1	A	276	PRO	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	98	MET	3.7
1	A	267	PRO	3.7
1	A	256	ARG	3.7
2	B	89	GLN	3.7
2	B	92	ILE	3.7
1	A	4	SER	3.6
1	A	25	VAL	3.6
1	A	247	VAL	3.6
2	B	85	VAL	3.6
2	B	60	TRP	3.6
2	B	17	ASN	3.6
1	A	104	GLY	3.6
1	A	265	GLY	3.6
1	A	28	VAL	3.6
1	A	56	GLY	3.5
2	B	80	CYS	3.5
1	A	100	GLY	3.5
1	A	216	THR	3.4
2	B	71	THR	3.4
1	A	58	GLU	3.4
1	A	106	ASP	3.4
2	B	76	ASP	3.4
1	A	60	TRP	3.4
2	B	79	ALA	3.3
1	A	65	GLN	3.3
1	A	164	CYS	3.3
1	A	110	LEU	3.3
1	A	261	VAL	3.3
2	B	98	ASP	3.2
1	A	163	LEU	3.2
1	A	250	PRO	3.2
1	A	99	TYR	3.2
2	B	65	LEU	3.2
1	A	275	GLU	3.2
2	B	42	ASN	3.2
1	A	8	PHE	3.2
1	A	26	GLY	3.2
2	B	18	GLY	3.2
2	B	7	ILE	3.2
1	A	7	TYR	3.2
1	A	153	ALA	3.1
1	A	74	TYR	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	42	SER	3.1
1	A	54	GLN	3.1
1	A	11	ALA	3.1
1	A	41	ALA	3.1
1	A	227	ASP	3.1
2	B	94	LYS	3.1
1	A	101	CYS	3.1
1	A	252	GLY	3.1
1	A	228	THR	3.1
1	A	142	ILE	3.0
1	A	165	VAL	3.0
1	A	241	PHE	3.0
2	B	22	PHE	3.0
2	B	36	GLU	3.0
2	B	73	THR	3.0
3	C	6	ALA	3.0
1	A	268	LYS	3.0
2	B	64	LEU	3.0
1	A	248	VAL	3.0
2	B	67	TYR	3.0
2	B	14	PRO	3.0
3	C	4	GLY	3.0
1	A	262	GLN	3.0
1	A	1	GLY	3.0
1	A	108	ARG	3.0
1	A	205	ALA	3.0
2	B	24	ASN	3.0
1	A	34	VAL	2.9
2	B	37	VAL	2.9
1	A	151	ARG	2.9
1	A	22	PHE	2.9
2	B	30	PHE	2.9
1	A	49	ALA	2.9
2	B	25	CYS	2.9
1	A	195	SER	2.9
3	C	7	ASP	2.9
1	A	52	ILE	2.9
2	B	54	LEU	2.9
1	A	211	ALA	2.9
1	A	51	TRP	2.9
2	B	47	GLU	2.9
2	B	70	PHE	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	264	GLU	2.8
1	A	213	ILE	2.8
1	A	221	GLY	2.8
1	A	10	THR	2.8
1	A	251	SER	2.8
1	A	222	GLU	2.8
2	B	27	VAL	2.8
2	B	57	SER	2.7
1	A	159	TYR	2.7
1	A	36	PHE	2.7
1	A	121	LYS	2.7
1	A	64	THR	2.7
1	A	61	ASP	2.7
1	A	27	TYR	2.7
1	A	199	ALA	2.7
2	B	16	GLU	2.7
2	B	48	LYS	2.7
1	A	31	THR	2.7
1	A	73	THR	2.7
1	A	223	ASP	2.7
1	A	94	ILE	2.7
2	B	83	ASN	2.7
1	A	40	ALA	2.7
1	A	182	ALA	2.7
1	A	204	TRP	2.7
1	A	92	SER	2.7
2	B	77	GLU	2.7
1	A	189	VAL	2.7
1	A	112	GLY	2.6
2	B	56	PHE	2.6
1	A	168	LEU	2.6
1	A	270	LEU	2.6
2	B	49	VAL	2.6
2	B	44	GLU	2.6
2	B	62	PHE	2.6
1	A	20	PRO	2.6
1	A	43	PRO	2.6
1	A	230	LEU	2.6
3	C	8	TYR	2.6
1	A	210	PRO	2.6
1	A	244	TRP	2.6
1	A	274	TRP	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	160	LEU	2.6
1	A	201	LEU	2.6
1	A	138	THR	2.6
1	A	187	THR	2.6
1	A	184	PRO	2.5
2	B	52	SER	2.5
1	A	185	PRO	2.5
1	A	198	GLU	2.5
1	A	44	ARG	2.5
1	A	136	ALA	2.5
1	A	154	GLU	2.5
2	B	78	TYR	2.5
1	A	95	ILE	2.5
2	B	95	TRP	2.5
1	A	178	THR	2.5
2	B	68	THR	2.5
1	A	57	PRO	2.5
1	A	219	ARG	2.4
2	B	29	GLY	2.4
1	A	226	GLN	2.4
1	A	186	LYS	2.4
1	A	85	TYR	2.4
1	A	209	TYR	2.4
2	B	35	ILE	2.4
1	A	249	VAL	2.4
1	A	3	HIS	2.4
1	A	215	LEU	2.4
1	A	155	GLN	2.4
1	A	257	TYR	2.3
2	B	15	ALA	2.3
2	B	33	SER	2.3
1	A	238	ASP	2.3
1	A	255	GLN	2.3
1	A	45	THR	2.3
2	B	4	THR	2.3
2	B	86	THR	2.3
1	A	113	HIS	2.3
1	A	150	ALA	2.3
1	A	145	ARG	2.3
1	A	220	ASP	2.3
1	A	71	THR	2.3
1	A	12	MET	2.3

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Mol	Chain	Res	Type	RSRZ
2	B	26	TYR	2.3
3	C	11	TYR	2.3
1	A	135	ALA	2.3
1	A	79	ARG	2.3
1	A	38	SER	2.3
1	A	88	SER	2.3
2	B	88	SER	2.3
1	A	229	GLU	2.3
3	C	1	HIS	2.3
1	A	69	THR	2.3
1	A	214	THR	2.3
1	A	23	ILE	2.2
1	A	66	ILE	2.2
2	B	81	ARG	2.2
1	A	272	LEU	2.2
1	A	90	ALA	2.2
1	A	231	VAL	2.2
1	A	76	GLU	2.2
1	A	172	LEU	2.2
1	A	237	GLY	2.2
2	B	11	SER	2.2
1	A	236	ALA	2.2
2	B	93	VAL	2.2
1	A	225	THR	2.2
1	A	240	THR	2.2
2	B	53	ASP	2.2
1	A	116	SER	2.2
1	A	117	ALA	2.2
2	B	41	LYS	2.2
2	B	10	TYR	2.1
1	A	59	TYR	2.1
2	B	96	ASP	2.1
1	A	167	TRP	2.1
1	A	62	ARG	2.1
1	A	152	VAL	2.1
1	A	78	LEU	2.1
1	A	102	ASP	2.1
2	B	63	TYR	2.1
1	A	48	ARG	2.1
1	A	217	TRP	2.1
2	B	51	HIS	2.1
1	A	63	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
3	C	3	VAL	2.1
1	A	130	LEU	2.1
1	A	179	LEU	2.1
1	A	203	CYS	2.1
2	B	23	LEU	2.1
1	A	29	ASP	2.1
1	A	119	ASP	2.1
1	A	97	ARG	2.1
2	B	50	GLU	2.0
1	A	77	SER	2.0
1	A	5	MET	2.0
1	A	224	GLN	2.0
1	A	235	PRO	2.0
1	A	147	TRP	2.0
2	B	40	LEU	2.0
1	A	33	PHE	2.0
1	A	18	GLY	2.0
1	A	115	GLN	2.0
1	A	143	THR	2.0
1	A	80	ASN	2.0
1	A	171	TYR	2.0
2	B	9	VAL	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 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.