



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 09:01 PM UTC

PDB ID : 6P2S / pdb_00006p2s
Title : Structure of a nested set of N-terminally extended MHC I-peptides provide novel insights into antigen processing and presentation
Authors : Li, L.; Batliwala, M.; Bouvier, M.
Deposited on : 2019-05-22
Resolution : 1.65 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

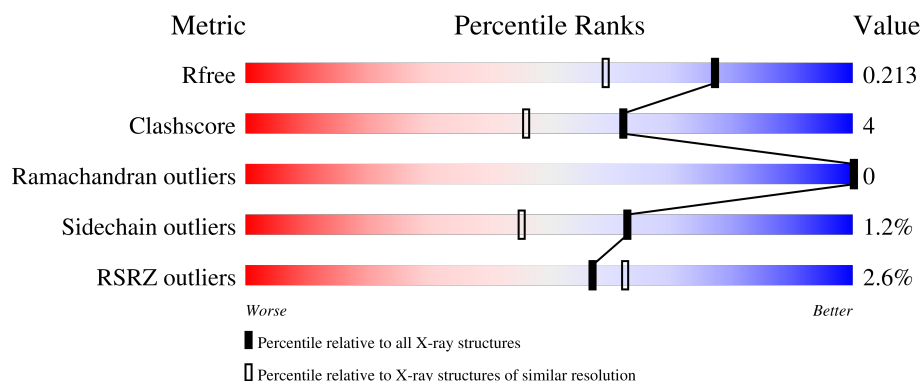
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.65 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	2563 (1.66-1.66)
Clashscore	190562	2662 (1.66-1.66)
Ramachandran outliers	187476	2621 (1.66-1.66)
Sidechain outliers	187428	2621 (1.66-1.66)
RSRZ outliers	180081	2564 (1.66-1.66)

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	3% 70% 26% .
2	B	100	2% 75% 23% .
3	C	11	9% 64% 18% 18%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 3390 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
1	A	275	Total	C	N	O	S	0	0	0
			2241	1388	410	435	8			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	76	CYS	GLU	engineered mutation	UNP R4ZGR5

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	100	Total	C	N	O	S	0	0	0
			837	533	141	159	4			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	MET	-	initiating methionine	UNP P61769

- Molecule 3 is a protein called MHC I-peptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	9	Total	C	N	O	S	0	0	0
			69	45	12	11	1			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	197	Total	O	0	0
			197	197		
4	B	39	Total	O	0	0
			39	39		

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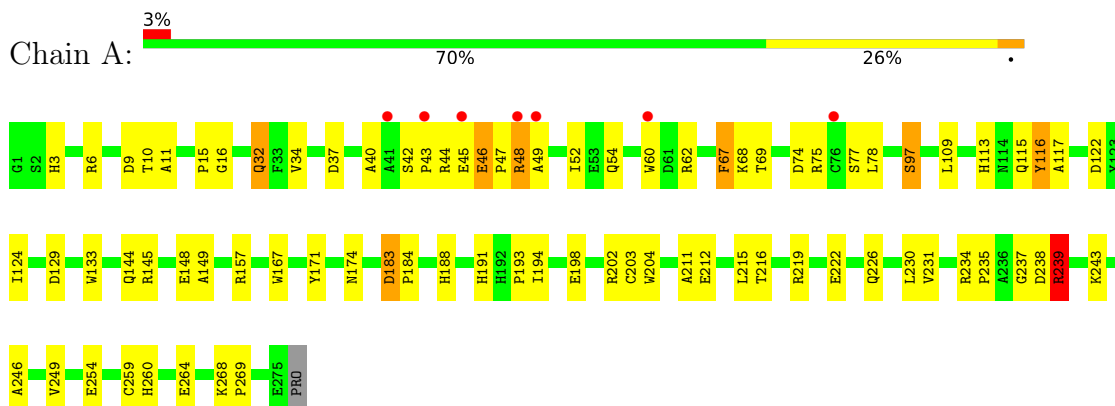
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	7	Total	O	0	0
			7	7		

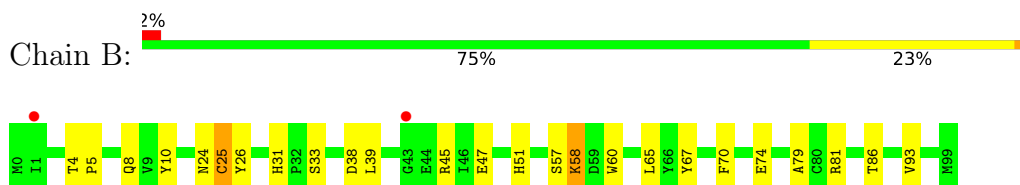
3 Residue-property plots

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.

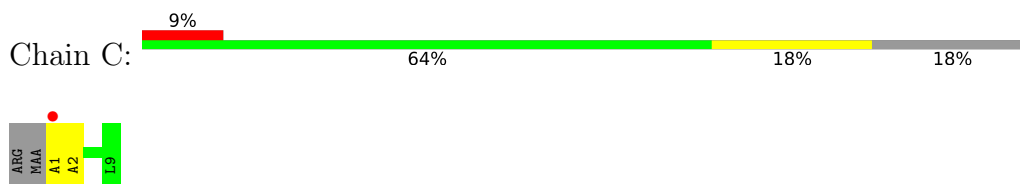
- Molecule 1: MHC class I antigen



- Molecule 2: Beta-2-microglobulin



- Molecule 3: MHC I-peptide



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	50.55Å 80.91Å 108.71Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	64.91 – 1.65 64.91 – 1.65	Depositor EDS
% Data completeness (in resolution range)	98.9 (64.91-1.65) 98.9 (64.91-1.65)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.04 (at 1.65Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.204 , 0.214 0.204 , 0.213	Depositor DCC
R_{free} test set	2694 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	26.0	Xtriage
Anisotropy	0.255	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 37.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	3390	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.33% 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

5.1 Standard geometry

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	2.10	66/2302 (2.9%)	1.38	3/3130 (0.1%)
2	B	1.96	18/860 (2.1%)	1.27	0/1162
3	C	1.80	0/69	1.57	2/88 (2.3%)
All	All	2.06	84/3231 (2.6%)	1.35	5/4380 (0.1%)

All (84) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	239	ARG	CD-NE	-11.33	1.30	1.46
1	A	184	PRO	CA-C	-8.79	1.44	1.52
1	A	260	HIS	CG-CD2	8.59	1.45	1.35
2	B	26	TYR	CA-C	-8.29	1.42	1.52
1	A	260	HIS	ND1-CE1	8.10	1.40	1.32
2	B	67	TYR	N-CA	7.81	1.55	1.45
1	A	188	HIS	CE1-NE2	7.57	1.40	1.32
1	A	145	ARG	CA-C	-7.50	1.43	1.52
2	B	31	HIS	ND1-CE1	7.44	1.40	1.32
2	B	79	ALA	N-CA	-7.38	1.37	1.46
2	B	57	SER	CA-CB	7.37	1.64	1.53
1	A	149	ALA	N-CA	7.34	1.55	1.46
2	B	31	HIS	CE1-NE2	7.32	1.39	1.32
2	B	24	ASN	CA-C	-7.27	1.44	1.52
2	B	10	TYR	CA-C	-7.23	1.44	1.52
1	A	246	ALA	N-CA	7.14	1.54	1.45
1	A	68	LYS	CA-CB	7.06	1.64	1.53
1	A	32	GLN	C-O	7.04	1.32	1.23
1	A	237	GLY	N-CA	7.01	1.55	1.45
1	A	37	ASP	CA-C	6.99	1.60	1.52
1	A	203	CYS	CA-C	6.96	1.61	1.52
1	A	67	PHE	N-CA	6.93	1.54	1.46
1	A	3	HIS	ND1-CE1	6.78	1.39	1.32
1	A	149	ALA	CA-C	-6.71	1.44	1.52
1	A	222	GLU	C-O	-6.70	1.16	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	269	PRO	N-CA	6.66	1.55	1.47
2	B	8	GLN	CA-C	-6.62	1.44	1.52
1	A	268	LYS	CA-C	6.56	1.59	1.52
1	A	234	ARG	CA-CB	6.48	1.63	1.54
1	A	122	ASP	CA-C	-6.46	1.44	1.52
1	A	144	GLN	N-CA	6.40	1.53	1.46
1	A	184	PRO	C-N	6.37	1.42	1.33
1	A	115	GLN	N-CA	-6.35	1.37	1.45
1	A	97	SER	CB-OG	-6.31	1.29	1.42
1	A	69	THR	CB-OG1	6.30	1.53	1.43
1	A	198	GLU	N-CA	6.27	1.53	1.45
1	A	16	GLY	N-CA	6.24	1.54	1.45
1	A	133	TRP	N-CA	6.23	1.53	1.45
1	A	183	ASP	CA-C	6.21	1.59	1.52
1	A	193	PRO	C-O	-6.12	1.16	1.23
1	A	78	LEU	C-O	-6.11	1.16	1.24
1	A	74	ASP	N-CA	6.11	1.53	1.46
1	A	129	ASP	CA-C	-6.10	1.44	1.52
1	A	109	LEU	C-O	5.94	1.31	1.23
1	A	249	VAL	CA-C	5.93	1.59	1.52
1	A	259	CYS	N-CA	5.93	1.53	1.46
2	B	33	SER	N-CA	-5.91	1.38	1.46
1	A	219	ARG	N-CA	5.88	1.53	1.46
1	A	202	ARG	N-CA	5.87	1.53	1.46
1	A	212	GLU	C-N	5.81	1.39	1.33
1	A	215	LEU	CB-CG	-5.80	1.41	1.53
1	A	157	ARG	NE-CZ	5.78	1.39	1.33
1	A	75	ARG	N-CA	5.75	1.53	1.46
1	A	204	TRP	CA-C	-5.74	1.45	1.52
1	A	11	ALA	CA-CB	-5.74	1.43	1.53
1	A	116	TYR	N-CA	5.59	1.52	1.45
1	A	15	PRO	C-N	-5.58	1.25	1.33
1	A	226	GLN	N-CA	-5.55	1.39	1.46
1	A	254	GLU	N-CA	5.55	1.53	1.46
1	A	188	HIS	CG-CD2	5.54	1.42	1.35
2	B	47	GLU	N-CA	5.51	1.53	1.46
1	A	216	THR	C-N	5.49	1.40	1.33
1	A	124	ILE	N-CA	5.48	1.52	1.46
2	B	47	GLU	CA-CB	5.47	1.62	1.53
2	B	25	CYS	N-CA	-5.44	1.40	1.46
1	A	3	HIS	CE1-NE2	5.43	1.38	1.32
1	A	191	HIS	N-CA	5.40	1.52	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	46	GLU	C-O	5.36	1.30	1.24
1	A	235	PRO	CA-CB	5.35	1.60	1.53
1	A	77	SER	CB-OG	5.32	1.52	1.42
1	A	167	TRP	CD2-CE2	5.31	1.50	1.41
1	A	148	GLU	N-CA	5.27	1.52	1.46
1	A	9	ASP	N-CA	5.22	1.52	1.46
1	A	211	ALA	N-CA	5.22	1.53	1.46
2	B	51	HIS	CE1-NE2	5.21	1.37	1.32
1	A	231	VAL	N-CA	-5.17	1.40	1.46
1	A	10	THR	C-O	5.14	1.29	1.24
2	B	58	LYS	C-N	5.13	1.40	1.33
1	A	113	HIS	CD2-NE2	5.09	1.43	1.37
1	A	264	GLU	N-CA	5.08	1.52	1.46
1	A	239	ARG	N-CA	5.06	1.52	1.46
2	B	81	ARG	CA-C	5.06	1.58	1.52
2	B	93	VAL	CA-CB	5.04	1.60	1.54
2	B	65	LEU	N-CA	5.01	1.52	1.46

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	239	ARG	NE-CZ-NH2	-7.88	112.10	119.20
3	C	1	ALA	CA-C-N	-5.86	111.40	120.31
3	C	1	ALA	C-N-CA	-5.86	111.40	120.31
1	A	194	ILE	CB-CA-C	-5.63	105.16	111.80
1	A	48	ARG	N-CA-C	-5.30	105.66	113.61

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	2241	0	2084	20	0
2	B	837	0	803	8	0
3	C	69	0	80	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	197	0	0	0	0
4	B	39	0	0	0	0
4	C	7	0	0	0	0
All	All	3390	0	2967	25	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 (25) 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:45:GLU:HG3	1:A:67:PHE:HE2	1.34	0.92
1:A:44:ARG:NH2	1:A:46:GLU:OE2	2.21	0.73
1:A:49:ALA:O	1:A:52:ILE:HG22	1.89	0.73
1:A:45:GLU:OE1	1:A:60:TRP:CE3	2.43	0.70
2:B:4:THR:HG22	2:B:5:PRO:HD2	1.80	0.61
2:B:4:THR:HG23	2:B:86:THR:OG1	2.00	0.61
1:A:45:GLU:HG3	1:A:67:PHE:CE2	2.26	0.60
1:A:42:SER:O	1:A:44:ARG:HG3	2.01	0.60
1:A:47:PRO:HB3	1:A:60:TRP:CH2	2.38	0.59
1:A:230:LEU:HD22	1:A:243:LYS:HE3	1.89	0.54
1:A:40:ALA:O	1:A:43:PRO:HD3	2.08	0.52
1:A:171:TYR:OH	3:C:2:ALA:HB2	2.10	0.51
1:A:34:VAL:CG2	1:A:45:GLU:HG2	2.40	0.51
1:A:54:GLN:HE22	1:A:174:ASN:HB3	1.77	0.49
2:B:4:THR:CG2	2:B:5:PRO:HD2	2.45	0.47
1:A:6:ARG:HE	2:B:58:LYS:HZ1	1.62	0.47
1:A:47:PRO:HB3	1:A:60:TRP:HH2	1.79	0.45
1:A:238:ASP:OD1	1:A:238:ASP:C	2.56	0.45
1:A:6:ARG:HE	2:B:58:LYS:NZ	2.15	0.44
2:B:25:CYS:HB2	2:B:39:LEU:HD21	1.99	0.44
1:A:97:SER:HB3	1:A:116:TYR:CD2	2.54	0.42
1:A:117:ALA:HB2	2:B:60:TRP:CE2	2.55	0.42
1:A:183:ASP:OD2	1:A:239:ARG:NH1	2.53	0.41
2:B:38:ASP:OD1	2:B:45:ARG:HD2	2.20	0.41
1:A:32:GLN:OE1	1:A:48:ARG:HG3	2.21	0.41

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	273/276 (99%)	267 (98%)	6 (2%)	0	100	100
2	B	98/100 (98%)	97 (99%)	1 (1%)	0	100	100
3	C	7/11 (64%)	7 (100%)	0	0	100	100
All	All	378/387 (98%)	371 (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	234/235 (100%)	232 (99%)	2 (1%)	70	56
2	B	95/95 (100%)	93 (98%)	2 (2%)	47	24
3	C	6/7 (86%)	6 (100%)	0	100	100
All	All	335/337 (99%)	331 (99%)	4 (1%)	63	45

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	62	ARG
1	A	239	ARG
2	B	70	PHE
2	B	74	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	GLN
1	A	114	ASN
1	A	144	GLN
1	A	224	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	275/276 (99%)	0.25	7 (2%) 58 64	19, 29, 54, 67	0
2	B	100/100 (100%)	0.56	2 (2%) 65 70	21, 39, 58, 71	0
3	C	9/11 (81%)	0.85	1 (11%) 10 11	26, 30, 42, 60	0
All	All	384/387 (99%)	0.34	10 (2%) 57 62	19, 31, 56, 71	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	1	ALA	6.6
1	A	45	GLU	4.7
1	A	43	PRO	4.1
1	A	60	TRP	3.2
1	A	49	ALA	2.9
2	B	43	GLY	2.8
2	B	1	ILE	2.8
1	A	76	CYS	2.3
1	A	48	ARG	2.2
1	A	41	ALA	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 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.