



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 09:27 PM UTC

PDB ID : 8HSW / pdb_00008hsw
Title : CRYSTAL STRUCTURE OF BAT MHC CLASS I MYLU-B-67 FOR 2.1
ANGSTROM
Authors : Wang, S.Q.; Zhang, N.Z.
Deposited on : 2022-12-20
Resolution : 2.03 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

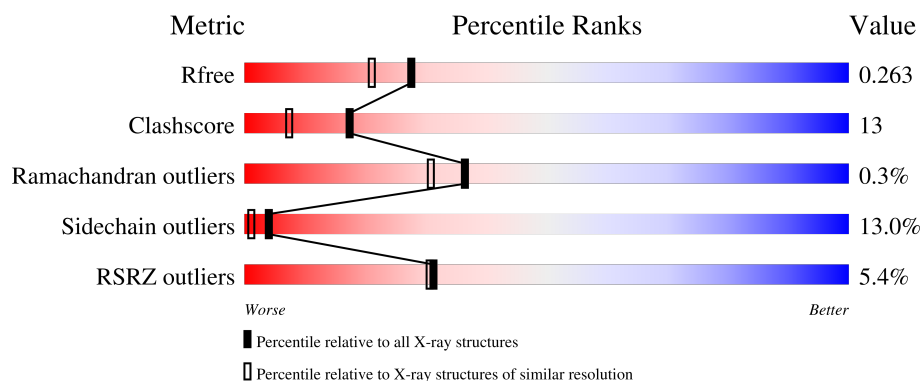
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.03 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	13299 (2.04-2.00)
Clashscore	190562	1022 (2.02-2.02)
Ramachandran outliers	187476	1014 (2.02-2.02)
Sidechain outliers	187428	1014 (2.02-2.02)
RSRZ outliers	180081	13314 (2.04-2.00)

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	280	8% 66% 28% 5%
2	B	97	74% 22% ..
3	C	9	100%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 3163 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 Ig-like domain-containing protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	280	Total	C	N	O	S	0	0	0
			2267	1428	403	428	8			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	97	Total	C	N	O	S	0	0	0
			800	509	138	149	4			

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1	GLU	-	expression tag	UNP L5K3Y9
B	2	PRO	-	expression tag	UNP L5K3Y9
B	3	ARG	-	expression tag	UNP L5K3Y9
B	96	ARG	-	expression tag	UNP L5K3Y9
B	97	ASN	-	expression tag	UNP L5K3Y9

- Molecule 3 is a protein called THR-PRO-GLN-SER-ALA-PRO-HIS-GLY-VAL.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	9	Total	C	N	O	0	0	0
			62	38	12	12			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	18	Total	O	0	0
			18	18		
4	B	15	Total	O	0	0
			15	15		

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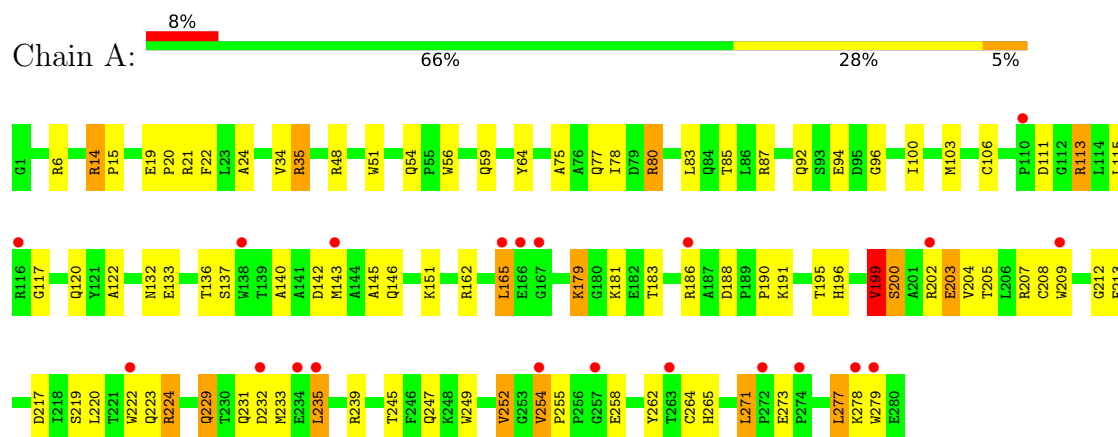
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	1	Total	O	0	0
			1	1		

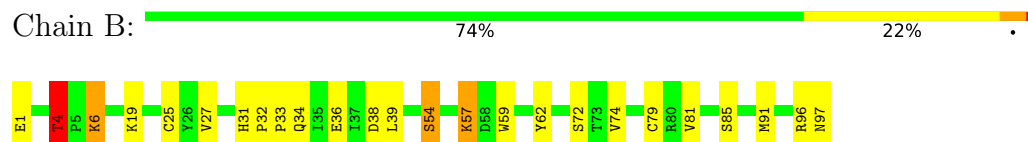
3 Residue-property plots [i](#)

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: Ig-like domain-containing protein



- Molecule 2: Beta-2-microglobulin



- Molecule 3: THR-PRO-GLN-SER-ALA-PRO-HIS-GLY-VAL



There are no outlier residues recorded for this chain.

4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	75.74Å 80.15Å 144.24Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.80 – 2.03 30.80 – 2.03	Depositor EDS
% Data completeness (in resolution range)	67.8 (30.80-2.03) 67.9 (30.80-2.03)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.25 (at 2.03Å)	Xtriage
Refinement program	REFMAC 5.8.0123	Depositor
R, R_{free}	0.234 , 0.262 0.241 , 0.263	Depositor DCC
R_{free} test set	1024 reflections (3.56%)	wwPDB-VP
Wilson B-factor (Å ²)	43.6	Xtriage
Anisotropy	0.030	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 21.0	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	0.93	EDS
Total number of atoms	3163	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.10% 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	1.05	3/2336 (0.1%)	1.48	12/3178 (0.4%)
2	B	0.97	0/826	1.28	1/1123 (0.1%)
3	C	1.03	0/64	1.39	0/88
All	All	1.03	3/3226 (0.1%)	1.43	13/4389 (0.3%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	273	GLU	C-N	12.22	1.50	1.33
1	A	271	LEU	C-N	7.12	1.50	1.33
1	A	209	TRP	C-O	-5.72	1.17	1.23

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	273	GLU	CA-C-N	13.26	133.44	119.78
1	A	273	GLU	C-N-CA	13.26	133.44	119.78
1	A	271	LEU	CA-C-N	11.30	133.97	119.84
1	A	271	LEU	C-N-CA	11.30	133.97	119.84
1	A	188	ASP	CB-CA-C	-6.24	102.73	109.85
1	A	195	THR	CA-CB-OG1	-6.15	100.38	109.60
1	A	199	VAL	CA-C-N	5.79	132.60	121.54
1	A	199	VAL	C-N-CA	5.79	132.60	121.54
1	A	142	ASP	CA-C-N	5.67	127.87	120.28
1	A	142	ASP	C-N-CA	5.67	127.87	120.28
1	A	273	GLU	O-C-N	-5.51	116.66	121.35
1	A	199	VAL	CA-C-O	-5.22	114.47	120.42
2	B	4	THR	CB-CA-C	5.10	117.67	109.41

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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	2267	0	2125	61	0
2	B	800	0	762	17	0
3	C	62	0	60	0	0
4	A	18	0	0	1	0
4	B	15	0	0	3	0
4	C	1	0	0	0	0
All	All	3163	0	2947	76	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 13.

All (76) 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:264:CYS:HB3	1:A:277:LEU:CD1	2.00	0.91
1:A:117:GLY:HA3	1:A:165:LEU:HD11	1.51	0.88
1:A:103:MET:HE3	1:A:120:GLN:HE21	1.43	0.84
2:B:1:GLU:HA	4:B:115:HOH:O	1.84	0.77
1:A:111:ASP:OD2	1:A:113:ARG:HB2	1.87	0.73
1:A:235:LEU:HD23	1:A:235:LEU:O	1.89	0.73
1:A:122:ALA:HB2	2:B:59:TRP:CE2	2.25	0.72
1:A:35:ARG:HG2	1:A:48:ARG:HD3	1.74	0.68
1:A:75:ALA:O	1:A:78:ILE:HG22	1.93	0.67
2:B:6:LYS:HA	2:B:6:LYS:HE2	1.77	0.67
1:A:77:GLN:HE22	1:A:80:ARG:NH1	1.94	0.65
2:B:31:HIS:CD2	2:B:32:PRO:HA	2.32	0.65
1:A:224:ARG:HB2	1:A:229:GLN:HE22	1.61	0.64
1:A:117:GLY:CA	1:A:165:LEU:HD11	2.27	0.63
1:A:199:VAL:O	1:A:199:VAL:HG13	2.01	0.60
2:B:57:LYS:HE3	2:B:57:LYS:H	1.66	0.60
1:A:35:ARG:HG2	1:A:48:ARG:CD	2.31	0.59
2:B:1:GLU:HG2	2:B:1:GLU:O	2.05	0.57
1:A:264:CYS:HB3	1:A:277:LEU:HD12	1.87	0.56
1:A:106:CYS:HB3	1:A:165:LEU:HD21	1.88	0.56
1:A:196:HIS:CE1	1:A:204:VAL:HG21	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:132:ASN:HD22	1:A:137:SER:HB3	1.71	0.55
1:A:223:GLN:HG3	1:A:265:HIS:CD2	2.41	0.55
1:A:133:GLU:O	1:A:133:GLU:HG2	2.07	0.55
1:A:146:GLN:NE2	1:A:146:GLN:HA	2.23	0.53
1:A:117:GLY:HA3	1:A:165:LEU:CD1	2.34	0.52
1:A:224:ARG:HB2	1:A:229:GLN:NE2	2.24	0.52
2:B:36:GLU:O	2:B:81:VAL:HA	2.09	0.52
1:A:207:ARG:HD3	1:A:249:TRP:CE3	2.45	0.51
1:A:277:LEU:HD12	1:A:277:LEU:H	1.75	0.51
1:A:277:LEU:HD12	1:A:277:LEU:N	2.23	0.51
2:B:32:PRO:HB2	2:B:33:PRO:HD2	1.91	0.51
1:A:19:GLU:OE1	1:A:80:ARG:NH2	2.45	0.50
1:A:77:GLN:HE22	1:A:80:ARG:HH11	1.59	0.50
1:A:136:THR:HG23	1:A:162:ARG:NH1	2.27	0.50
1:A:202:ARG:O	1:A:255:PRO:HA	2.12	0.49
1:A:15:PRO:HG2	1:A:96:GLY:O	2.13	0.49
1:A:6:ARG:HD2	1:A:103:MET:SD	2.53	0.49
1:A:106:CYS:HB3	1:A:165:LEU:CD2	2.42	0.49
1:A:264:CYS:HB3	1:A:277:LEU:HD11	1.93	0.48
1:A:136:THR:CG2	1:A:162:ARG:HH11	2.27	0.48
1:A:14:ARG:NH1	1:A:21:ARG:HB2	2.29	0.47
2:B:4:THR:HA	2:B:85:SER:OG	2.14	0.47
1:A:196:HIS:HB2	1:A:279:TRP:CH2	2.51	0.46
1:A:132:ASN:ND2	1:A:137:SER:HB3	2.31	0.46
1:A:233:MET:HB2	1:A:252:VAL:HG13	1.98	0.45
1:A:122:ALA:HB2	2:B:59:TRP:CD2	2.50	0.45
1:A:83:LEU:HD21	1:A:100:ILE:HG22	1.99	0.45
2:B:19:LYS:NZ	4:B:102:HOH:O	2.48	0.45
1:A:190:PRO:HD2	1:A:271:LEU:HG	1.99	0.44
2:B:25:CYS:HB2	2:B:39:LEU:HD21	1.99	0.44
1:A:140:ALA:HB1	1:A:145:ALA:CB	2.48	0.44
1:A:146:GLN:HA	1:A:146:GLN:HE21	1.81	0.44
1:A:203:GLU:HA	1:A:254:VAL:O	2.17	0.44
1:A:207:ARG:HD2	1:A:249:TRP:CG	2.52	0.44
1:A:224:ARG:HG3	1:A:262:TYR:CZ	2.53	0.44
2:B:79:CYS:O	2:B:91:MET:HA	2.18	0.43
2:B:57:LYS:H	2:B:57:LYS:CE	2.30	0.43
1:A:19:GLU:HB3	1:A:20:PRO:HD2	1.99	0.43
1:A:224:ARG:HB2	1:A:229:GLN:OE1	2.19	0.42
2:B:38:ASP:HA	4:B:109:HOH:O	2.19	0.42
1:A:35:ARG:HG2	1:A:48:ARG:CG	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:239:ARG:HG2	1:A:247:GLN:HB2	2.02	0.41
2:B:54:SER:HB3	2:B:62:TYR:CZ	2.55	0.41
1:A:51:TRP:HA	1:A:54:GLN:CD	2.46	0.41
1:A:208:CYS:HB2	1:A:222:TRP:CZ2	2.55	0.41
1:A:64:TYR:CD1	1:A:64:TYR:C	2.99	0.41
2:B:4:THR:HG22	2:B:85:SER:HB2	2.03	0.41
1:A:103:MET:CE	1:A:120:GLN:HE21	2.24	0.41
1:A:22:PHE:CE1	1:A:24:ALA:HB2	2.56	0.41
1:A:56:TRP:CG	1:A:179:LYS:HG3	2.56	0.41
1:A:212:GLY:HA2	1:A:245:THR:OG1	2.21	0.41
1:A:87:ARG:NH1	1:A:92:GLN:O	2.55	0.40
1:A:190:PRO:CA	1:A:213:PHE:HB3	2.51	0.40
1:A:196:HIS:HB2	1:A:279:TRP:CZ3	2.57	0.40
1:A:219:SER:HA	4:A:309:HOH:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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	278/280 (99%)	260 (94%)	17 (6%)	1 (0%)	30	22
2	B	95/97 (98%)	92 (97%)	3 (3%)	0	100	100
3	C	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
All	All	380/386 (98%)	358 (94%)	21 (6%)	1 (0%)	36	31

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	200	SER

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	233/233 (100%)	200 (86%)	33 (14%)	3	1
2	B	91/91 (100%)	81 (89%)	10 (11%)	6	1
3	C	7/7 (100%)	7 (100%)	0	100	100
All	All	331/331 (100%)	288 (87%)	43 (13%)	4	1

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	ARG
1	A	34	VAL
1	A	35	ARG
1	A	59	GLN
1	A	80	ARG
1	A	85	THR
1	A	94	GLU
1	A	113	ARG
1	A	115	LEU
1	A	143	MET
1	A	151	LYS
1	A	165	LEU
1	A	179	LYS
1	A	181	LYS
1	A	183	THR
1	A	186	ARG
1	A	191	LYS
1	A	199	VAL
1	A	200	SER
1	A	203	GLU
1	A	205	THR
1	A	217	ASP
1	A	220	LEU
1	A	224	ARG
1	A	229	GLN
1	A	231	GLN

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Mol	Chain	Res	Type
1	A	232	ASP
1	A	235	LEU
1	A	252	VAL
1	A	254	VAL
1	A	258	GLU
1	A	277	LEU
1	A	278	LYS
2	B	4	THR
2	B	6	LYS
2	B	27	VAL
2	B	34	GLN
2	B	54	SER
2	B	57	LYS
2	B	72	SER
2	B	74	VAL
2	B	96	ARG
2	B	97	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	GLN
1	A	77	GLN
1	A	120	GLN
1	A	132	ASN
1	A	146	GLN
1	A	174	GLN
1	A	196	HIS
1	A	231	GLN
1	A	260	GLN
1	A	265	HIS
2	B	13	HIS
2	B	31	HIS
2	B	44	GLN
2	B	50	GLN
2	B	66	HIS
2	B	82	ASN

5.3.3 RNA ⓘ

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	280/280 (100%)	0.68	21 (7%) 20 19	29, 50, 78, 96	0
2	B	97/97 (100%)	0.10	0 100 100	27, 39, 56, 66	0
3	C	9/9 (100%)	0.17	0 100 100	36, 40, 44, 45	0
All	All	386/386 (100%)	0.52	21 (5%) 31 30	27, 46, 74, 96	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	235	LEU	6.0
1	A	165	LEU	3.6
1	A	254	VAL	3.6
1	A	257	GLY	3.2
1	A	143	MET	3.0
1	A	234	GLU	2.8
1	A	167	GLY	2.8
1	A	222	TRP	2.7
1	A	232	ASP	2.7
1	A	278	LYS	2.5
1	A	279	TRP	2.4
1	A	202	ARG	2.3
1	A	166	GLU	2.3
1	A	272	PRO	2.3
1	A	116	ARG	2.2
1	A	263	THR	2.2
1	A	110	PRO	2.1
1	A	138	TRP	2.1
1	A	186	ARG	2.1
1	A	209	TRP	2.0
1	A	274	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 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.