



wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 26, 2026 – 01:17 PM EDT

PDB ID : 8EN8 / pdb_00008en8
Title : Cross-reactive 3180 TCR recognition of HLA-B*35:01-NP4 epitope from 1972 influenza strain
Authors : Littler, D.R.; Rossjohn, J.
Deposited on : 2022-09-29
Resolution : 2.70 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

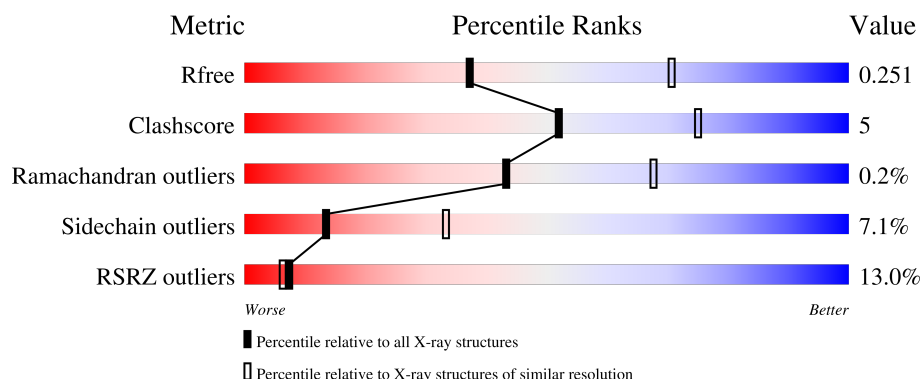
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	11% 88% 10% .
1	F	276	7% 88% 12% .
2	B	100	7% 92% 6% ..
2	G	100	2% 89% 9% ..
3	C	9	67% 33%

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Mol	Chain	Length	Quality of chain
3	H	9	56% 44%
4	D	205	2% 88% 11%
4	I	205	33% 86% 12% .
5	E	245	2% 80% 16% .
5	J	245	33% 75% 20% . .

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 13859 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	276	Total	C	N	O	S	0	1	0
			2262	1409	413	433	7			
1	F	276	Total	C	N	O	S	0	1	0
			2262	1409	413	433	7			

- 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			
2	G	99	Total	C	N	O	S	0	0	0
			829	528	140	158	3			

There are 2 discrepancies between the modelled and reference sequences:

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

- Molecule 3 is a protein called Nucleoprotein NP4 epitope.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	9	Total	C	N	O	S	0	0	0
			73	48	10	14	1			
3	H	9	Total	C	N	O	S	0	0	0
			73	48	10	14	1			

- Molecule 4 is a protein called 3180 TCR alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	205	Total	C	N	O	S	0	0	0
			1594	994	266	326	8			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	I	205	Total	C	N	O	S	0	0	0
			1594	994	266	326	8			

- Molecule 5 is a protein called 3180 TCR beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	245	Total	C	N	O	S	0	0	0
			1937	1219	334	375	9			
5	J	245	Total	C	N	O	S	0	0	0
			1937	1219	334	375	9			

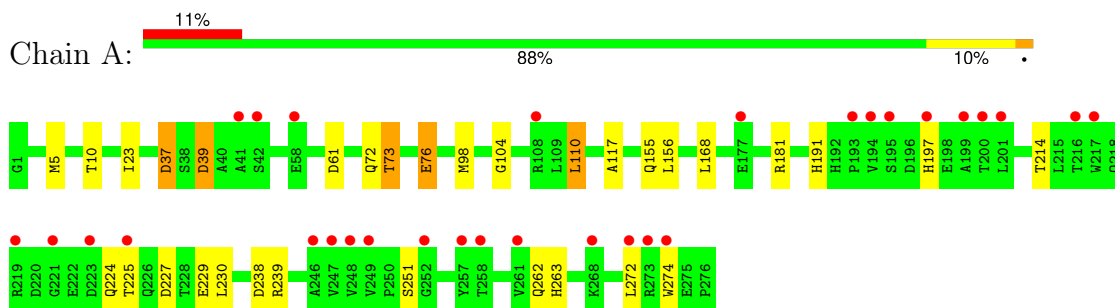
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	79	Total	O	0	0
			79	79		
6	B	14	Total	O	0	0
			14	14		
6	C	3	Total	O	0	0
			3	3		
6	D	51	Total	O	0	0
			51	51		
6	E	80	Total	O	0	0
			80	80		
6	F	110	Total	O	0	0
			110	110		
6	G	36	Total	O	0	0
			36	36		
6	H	8	Total	O	0	0
			8	8		
6	I	34	Total	O	0	0
			34	34		
6	J	54	Total	O	0	0
			54	54		

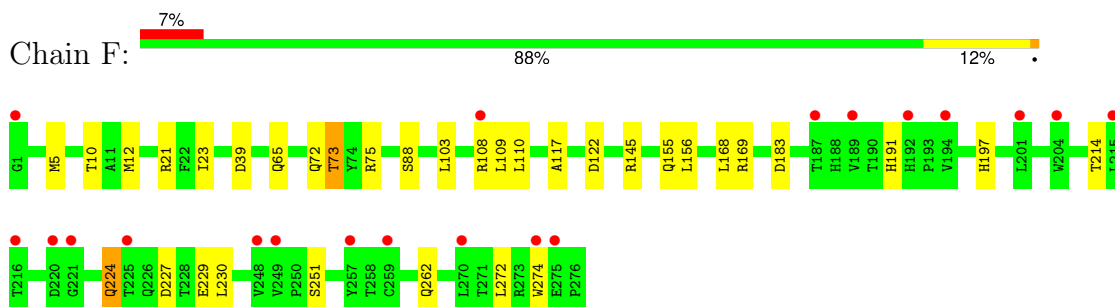
3 Residue-property plots [i](#)

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.

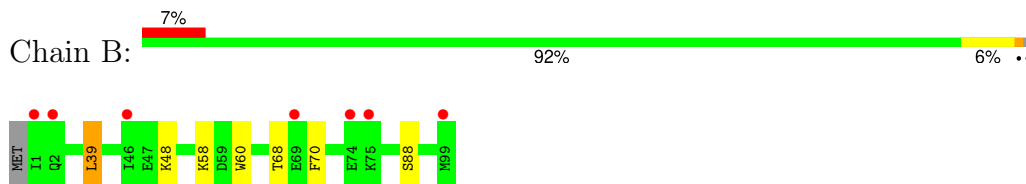
- Molecule 1: MHC class I antigen



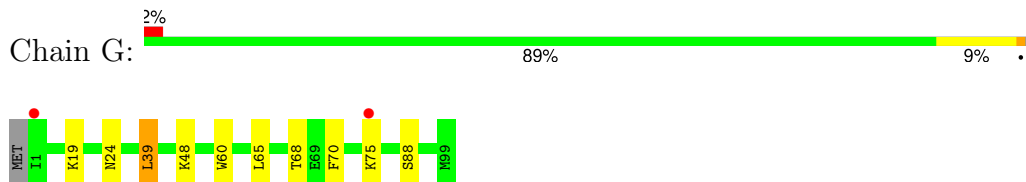
- Molecule 1: MHC class I antigen



- Molecule 2: Beta-2-microglobulin

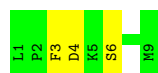


- Molecule 2: Beta-2-microglobulin



- Molecule 3: Nucleoprotein NP4 epitope

Chain C:  67% 33%



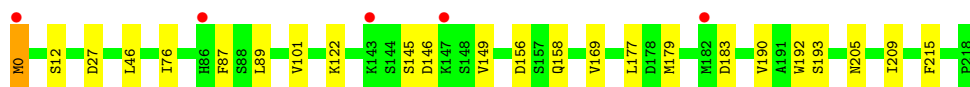
- Molecule 3: Nucleoprotein NP4 epitope

Chain H:  56% 44%



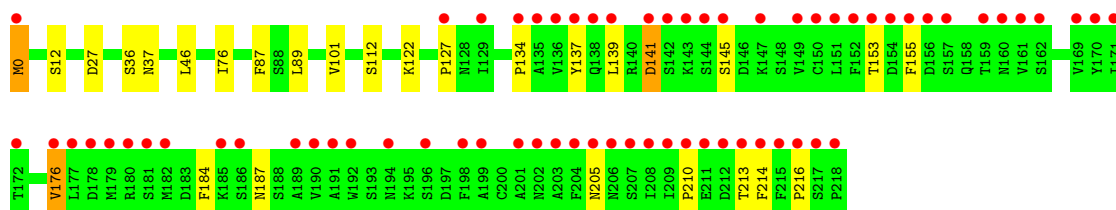
- Molecule 4: 3180 TCR alpha chain

Chain D:  2% 88% 11%



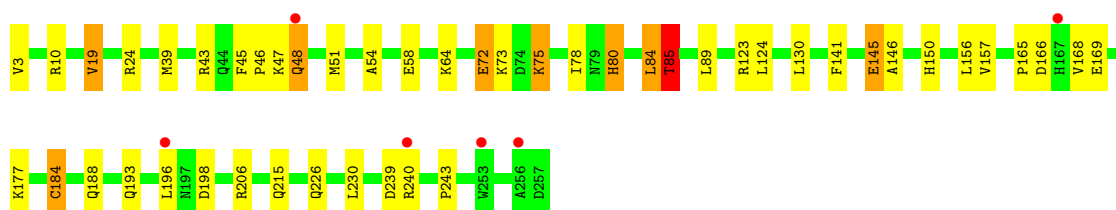
- Molecule 4: 3180 TCR alpha chain

Chain I:  33% 86% 12%



- Molecule 5: 3180 TCR beta chain

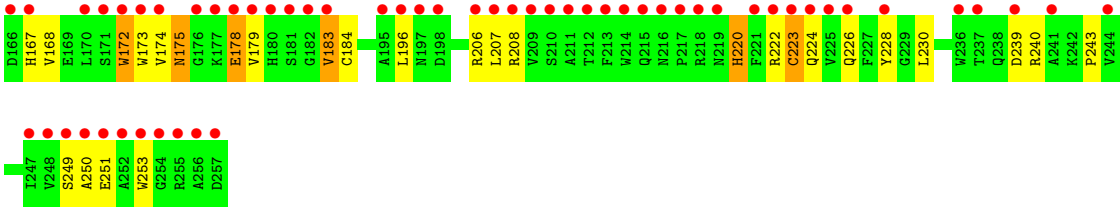
Chain E:  2% 80% 16%



- Molecule 5: 3180 TCR beta chain

Chain J:  33% 75% 20%





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	79.77Å 116.69Å 253.18Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	27.20 – 2.70 27.20 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.9 (27.20-2.70) 99.8 (27.20-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.12 (at 2.72Å)	Xtriage
Refinement program	BUSTER, PHENIX 1.10.1_2155	Depositor
R, R_{free}	0.207 , 0.249 0.211 , 0.251	Depositor DCC
R_{free} test set	3281 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	46.2	Xtriage
Anisotropy	0.458	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 76.3	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	0.92	EDS
Total number of atoms	13859	wwPDB-VP
Average B, all atoms (Å ²)	83.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.90% 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	0.79	3/2325 (0.1%)	1.21	4/3161 (0.1%)
1	F	0.80	1/2325 (0.0%)	1.22	7/3161 (0.2%)
2	B	0.75	0/852	1.10	1/1152 (0.1%)
2	G	0.73	0/852	1.12	1/1152 (0.1%)
3	C	1.15	0/74	1.23	1/97 (1.0%)
3	H	0.68	0/74	1.24	1/97 (1.0%)
4	D	0.72	0/1628	1.17	4/2205 (0.2%)
4	I	0.78	0/1628	1.16	2/2205 (0.1%)
5	E	0.69	0/1988	1.15	6/2705 (0.2%)
5	J	0.77	0/1988	1.17	5/2705 (0.2%)
All	All	0.76	4/13734 (0.0%)	1.18	32/18640 (0.2%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	23	ILE	C-O	-5.69	1.18	1.24
1	A	37	ASP	C-O	-5.22	1.18	1.23
1	F	23	ILE	C-O	-5.21	1.18	1.24
1	A	10	THR	C-O	-5.06	1.18	1.23

The worst 5 of 32 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	165	PRO	CA-C-N	6.44	131.00	120.63
5	E	165	PRO	C-N-CA	6.44	131.00	120.63
5	J	178	GLU	CB-CG-CD	6.12	123.01	112.60
3	H	4	ASP	CA-CB-CG	5.96	118.56	112.60
2	B	70	PHE	CA-CB-CG	5.90	119.70	113.80

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	2262	0	2122	14	0
1	F	2262	0	2122	10	0
2	B	829	0	794	3	0
2	G	829	0	794	3	0
3	C	73	0	78	2	0
3	H	73	0	78	3	0
4	D	1594	0	1521	8	0
4	I	1594	0	1521	27	0
5	E	1937	0	1856	30	0
5	J	1937	0	1856	59	0
6	A	79	0	0	0	0
6	B	14	0	0	0	0
6	C	3	0	0	0	0
6	D	51	0	0	0	0
6	E	80	0	0	2	0
6	F	110	0	0	0	0
6	G	36	0	0	0	0
6	H	8	0	0	0	0
6	I	34	0	0	1	0
6	J	54	0	0	0	0
All	All	13859	0	12742	132	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 5.

The worst 5 of 132 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)
5:J:147:GLU:O	5:J:148:ILE:CG1	1.95	1.14
5:J:147:GLU:O	5:J:148:ILE:HG12	1.52	1.06
5:J:147:GLU:C	5:J:148:ILE:HG12	1.77	1.06
4:I:127:PRO:HG3	4:I:176:VAL:HG11	1.40	1.03
5:J:175:ASN:H	5:J:220:HIS:HD2	1.08	1.00

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	275/276 (100%)	265 (96%)	9 (3%)	1 (0%)	30	54
1	F	275/276 (100%)	262 (95%)	12 (4%)	1 (0%)	30	54
2	B	97/100 (97%)	95 (98%)	2 (2%)	0	100	100
2	G	97/100 (97%)	96 (99%)	1 (1%)	0	100	100
3	C	7/9 (78%)	7 (100%)	0	0	100	100
3	H	7/9 (78%)	7 (100%)	0	0	100	100
4	D	203/205 (99%)	195 (96%)	8 (4%)	0	100	100
4	I	203/205 (99%)	191 (94%)	12 (6%)	0	100	100
5	E	243/245 (99%)	232 (96%)	10 (4%)	1 (0%)	30	54
5	J	243/245 (99%)	224 (92%)	18 (7%)	1 (0%)	30	54
All	All	1650/1670 (99%)	1574 (95%)	72 (4%)	4 (0%)	43	68

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	J	148	ILE
1	A	251	SER
5	E	166	ASP
1	F	251	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	235/234 (100%)	224 (95%)	11 (5%)	23	51
1	F	235/234 (100%)	222 (94%)	13 (6%)	19	45
2	B	94/95 (99%)	91 (97%)	3 (3%)	34	64
2	G	94/95 (99%)	89 (95%)	5 (5%)	20	46
3	C	9/9 (100%)	9 (100%)	0	100	100
3	H	9/9 (100%)	9 (100%)	0	100	100
4	D	182/182 (100%)	171 (94%)	11 (6%)	17	41
4	I	182/182 (100%)	173 (95%)	9 (5%)	22	49
5	E	216/216 (100%)	192 (89%)	24 (11%)	6	15
5	J	216/216 (100%)	187 (87%)	29 (13%)	4	9
All	All	1472/1472 (100%)	1367 (93%)	105 (7%)	13	33

5 of 105 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	183	ASP
4	I	76	ILE
5	J	220	HIS
1	F	229	GLU
2	G	75	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 25 such sidechains are listed below:

Mol	Chain	Res	Type
5	E	246	GLN
1	F	218	GLN
5	J	220	HIS
1	F	180	GLN
2	G	17	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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	276/276 (100%)	0.52	30 (10%) 10 9	20, 66, 177, 207	8 (2%)
1	F	276/276 (100%)	0.22	20 (7%) 21 18	17, 52, 185, 205	9 (3%)
2	B	99/100 (99%)	0.85	7 (7%) 22 19	47, 87, 127, 138	6 (6%)
2	G	99/100 (99%)	0.20	2 (2%) 65 62	32, 62, 99, 115	6 (6%)
3	C	9/9 (100%)	-0.60	0 100 100	29, 34, 43, 50	0
3	H	9/9 (100%)	-0.36	0 100 100	26, 32, 36, 39	0
4	D	205/205 (100%)	0.18	5 (2%) 59 56	32, 61, 105, 139	1 (0%)
4	I	205/205 (100%)	1.38	67 (32%) 1 1	32, 91, 226, 253	0
5	E	245/245 (100%)	0.13	6 (2%) 59 56	27, 57, 103, 144	0
5	J	245/245 (100%)	1.35	80 (32%) 1 1	27, 107, 230, 263	0
All	All	1668/1670 (99%)	0.59	217 (13%) 7 6	17, 66, 193, 263	30 (1%)

The worst 5 of 217 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	J	156	LEU	8.3
2	B	1	ILE	8.0
5	J	256	ALA	7.8
4	I	151	LEU	7.0
4	I	209	ILE	6.9

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.