



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 09:58 PM UTC

PDB ID : 4P5T / pdb_00004p5t
Title : 14.C6 TCR complexed with MHC class II I-Ab/3K peptide
Authors : Trenh, P.; Stadinski, B.; Huseby, E.S.; Stern, L.J.
Deposited on : 2014-03-19
Resolution : 3.26 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

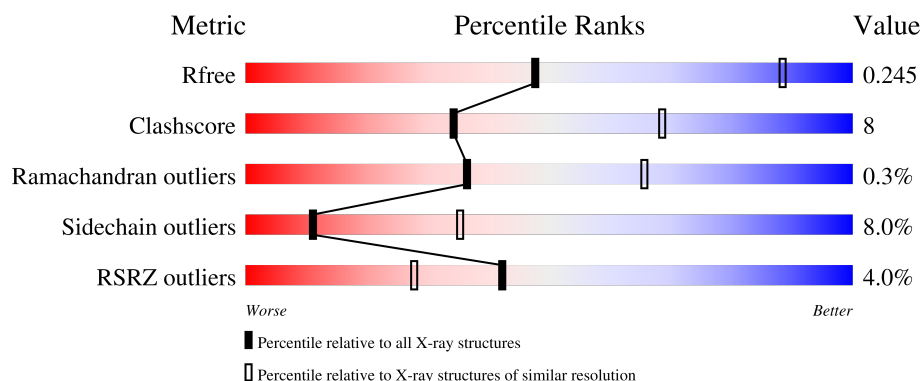
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.26 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	1605 (3.30-3.22)
Clashscore	190562	1660 (3.30-3.22)
Ramachandran outliers	187476	1630 (3.30-3.22)
Sidechain outliers	187428	1629 (3.30-3.22)
RSRZ outliers	180081	1605 (3.30-3.22)

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	206	77% 18% .
1	E	206	11% 69% 18% . 9%
2	B	241	76% 20% ..
2	F	241	10% 72% 22% . 5%
3	C	182	79% 19% ..

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Mol	Chain	Length	Quality of chain
3	G	182	3% 82% 16% ••
4	D	217	69% 21% • 8%
4	H	217	2% 69% 19% • 8%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12366 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 TRA protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	197	Total	C	N	O	S	0	0	0
			1488	948	241	292	7			
1	E	188	Total	C	N	O	S	0	0	0
			1403	902	223	272	6			

- Molecule 2 is a protein called Human nkt tcr beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	238	Total	C	N	O	S	0	0	0
			1815	1146	318	345	6			
2	F	229	Total	C	N	O	S	0	0	0
			1725	1091	300	328	6			

- Molecule 3 is a protein called H-2 class II histocompatibility antigen, A-B alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	179	Total	C	N	O	S	0	0	0
			1381	897	215	266	3			
3	G	179	Total	C	N	O	S	0	0	0
			1377	895	214	265	3			

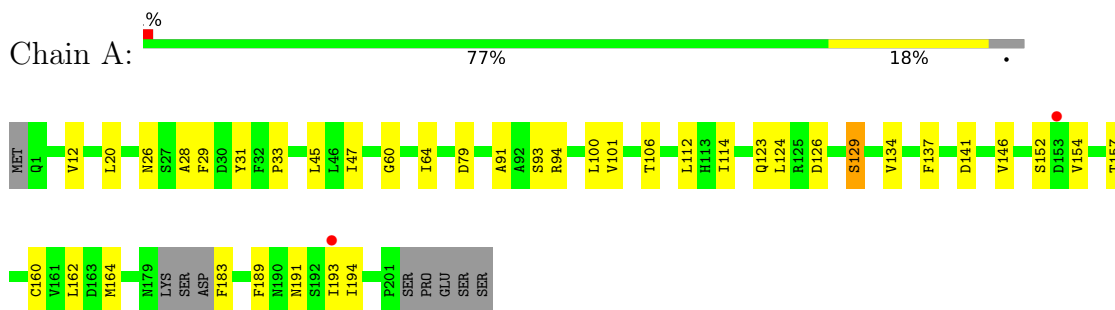
- Molecule 4 is a protein called protein of 3K peptide (FEAQKAKANKAVD), Linker region - GGGGSLVPRGSGGGG, H-2 class II histocompatibility antigen, A beta chain, H-2 class II histocompatibility antigen, A beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	199	Total	C	N	O	S	0	0	0
			1593	1001	279	307	6			
4	H	199	Total	C	N	O	S	0	0	0
			1584	997	275	306	6			

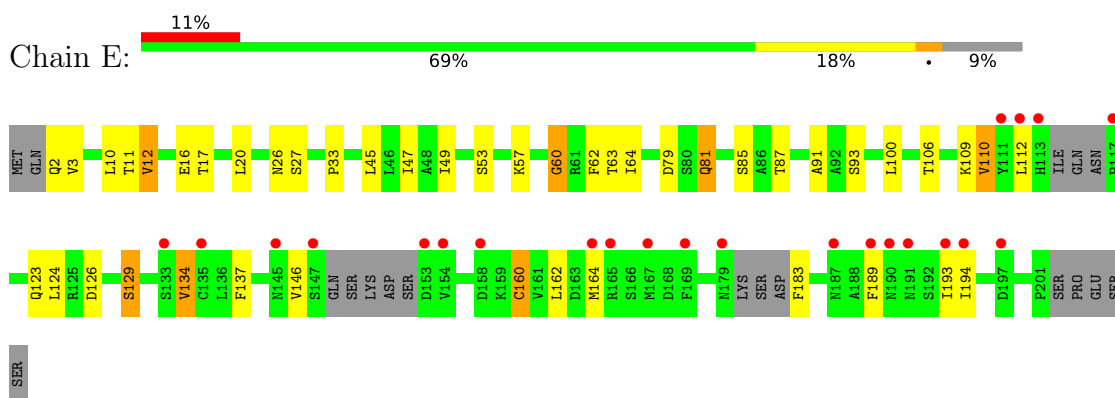
3 Residue-property plots [i](#)

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.

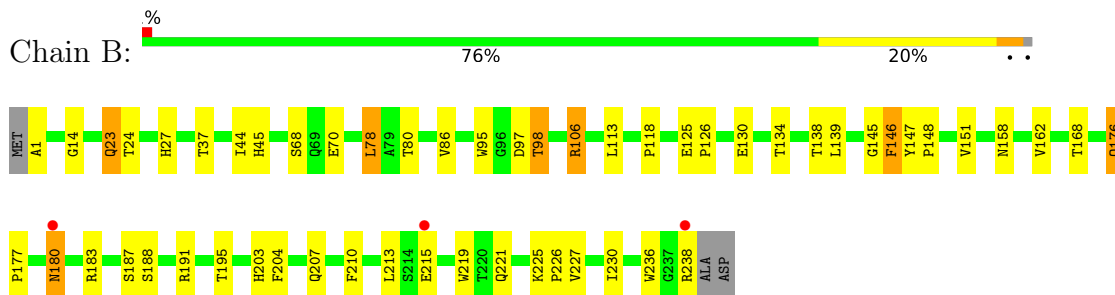
- Molecule 1: TRA protein



- Molecule 1: TRA protein

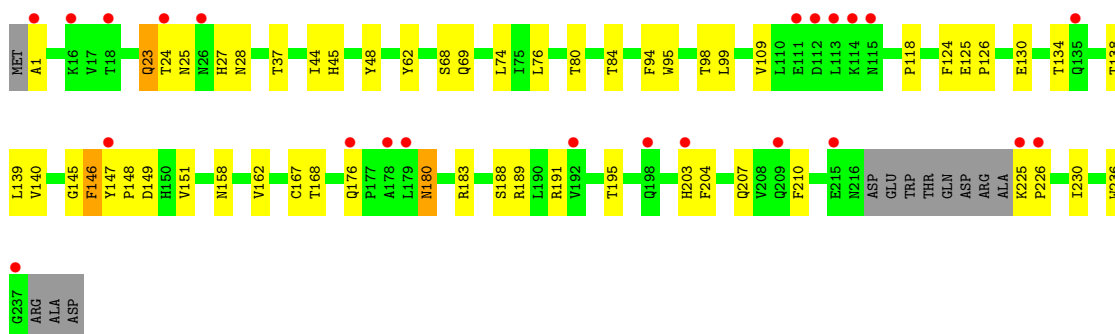


- Molecule 2: Human nkt tcr beta chain

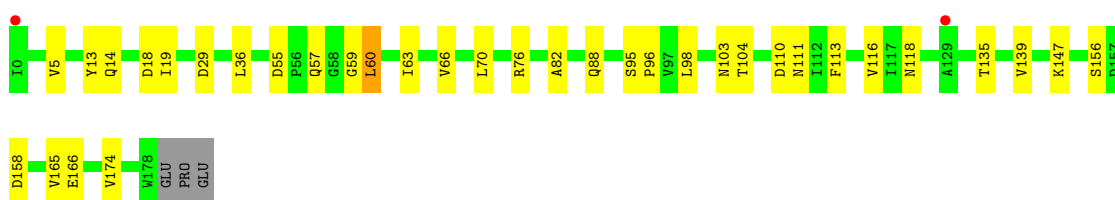
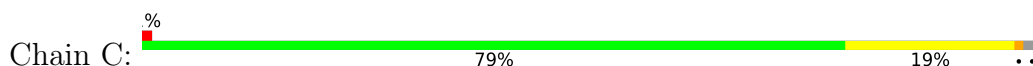


- Molecule 2: Human nkt tcr beta chain

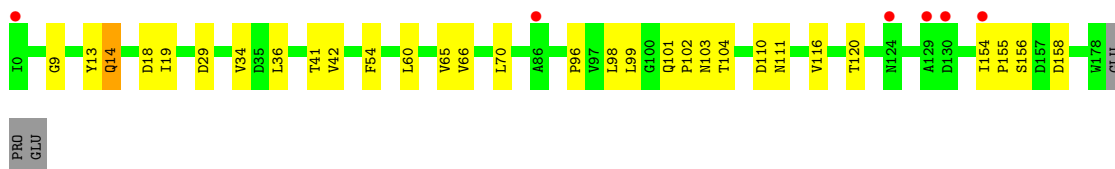
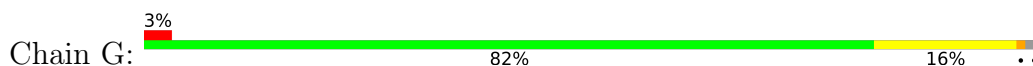




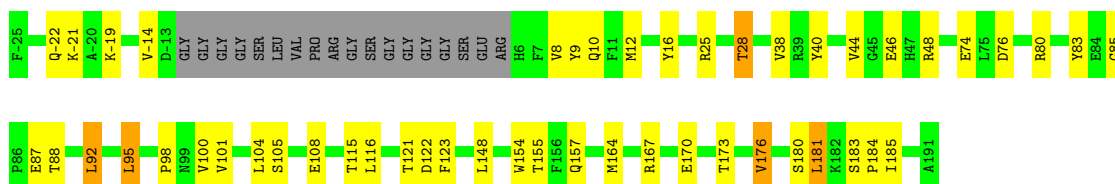
- Molecule 3: H-2 class II histocompatibility antigen, A-B alpha chain



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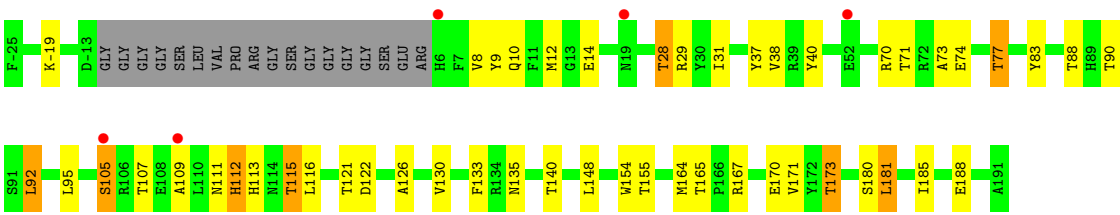


- Molecule 4: protein of 3K peptide (FEAQKAKANKAVD),Linker region - GGGGSLVPRGSGGGG,H-2 class II histocompatibility antigen, A beta chain,H-2 class II histocompatibility antigen, A beta chain



- Molecule 4: protein of 3K peptide (FEAQKAKANKAVD),Linker region - GGGGSLVPRGSGGGG,H-2 class II histocompatibility antigen, A beta chain,H-2 class II histocompatibility antigen, A beta chain





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	66.01Å 74.14Å 259.29Å 90.00° 92.00° 90.00°	Depositor
Resolution (Å)	47.05 – 3.26 47.05 – 3.26	Depositor EDS
% Data completeness (in resolution range)	99.0 (47.05-3.26) 98.9 (47.05-3.26)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.42 (at 3.25Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, R_{free}	0.186 , 0.236 0.201 , 0.245	Depositor DCC
R_{free} test set	1957 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	49.4	Xtriage
Anisotropy	0.433	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 72.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.024 for h,-k,-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	12366	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.45% 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	0.29	0/1525	0.70	0/2078
1	E	0.28	0/1438	0.67	0/1960
2	B	0.29	0/1868	0.76	2/2558 (0.1%)
2	F	0.27	0/1775	0.76	4/2432 (0.2%)
3	C	0.28	0/1425	0.71	0/1957
3	G	0.26	0/1420	0.70	0/1949
4	D	0.28	0/1632	0.72	2/2225 (0.1%)
4	H	0.28	0/1623	0.72	0/2214
All	All	0.28	0/12706	0.72	8/17373 (0.0%)

There are no bond length outliers.

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	176	GLN	CA-C-N	6.27	125.96	119.56
2	F	176	GLN	C-N-CA	6.27	125.96	119.56
2	B	176	GLN	CA-C-N	6.15	125.83	119.56
2	B	176	GLN	C-N-CA	6.15	125.83	119.56
2	F	125	GLU	CA-C-N	5.09	125.10	119.90

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	1488	0	1353	19	0
1	E	1403	0	1255	18	0
2	B	1815	0	1654	35	0
2	F	1725	0	1561	42	0
3	C	1381	0	1263	19	0
3	G	1377	0	1256	16	0
4	D	1593	0	1471	30	0
4	H	1584	0	1456	29	0
All	All	12366	0	11269	179	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 8.

The worst 5 of 179 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:F:84:THR:HG22	2:F:109:VAL:H	1.46	0.80
4:D:116:LEU:HG	4:D:164:MET:HE2	1.66	0.77
1:E:45:LEU:HD22	2:F:98:THR:HG22	1.69	0.74
2:B:130:GLU:OE2	2:B:191:ARG:NH1	2.20	0.74
2:F:130:GLU:OE2	2:F:191:ARG:NH1	2.20	0.74

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	193/206 (94%)	182 (94%)	9 (5%)	2 (1%)	12 40
1	E	180/206 (87%)	172 (96%)	6 (3%)	2 (1%)	11 38
2	B	236/241 (98%)	225 (95%)	11 (5%)	0	100 100
2	F	225/241 (93%)	213 (95%)	12 (5%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	177/182 (97%)	172 (97%)	5 (3%)	0	100	100
3	G	175/182 (96%)	168 (96%)	7 (4%)	0	100	100
4	D	195/217 (90%)	185 (95%)	9 (5%)	1 (0%)	24	55
4	H	195/217 (90%)	189 (97%)	6 (3%)	0	100	100
All	All	1576/1692 (93%)	1506 (96%)	65 (4%)	5 (0%)	36	66

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	60	GLY
1	E	60	GLY
1	E	79	ASP
1	A	79	ASP
4	D	105	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	157/185 (85%)	143 (91%)	14 (9%)	9	30
1	E	143/185 (77%)	120 (84%)	23 (16%)	2	11
2	B	185/206 (90%)	171 (92%)	14 (8%)	12	36
2	F	175/206 (85%)	165 (94%)	10 (6%)	18	46
3	C	147/163 (90%)	140 (95%)	7 (5%)	23	50
3	G	146/163 (90%)	138 (94%)	8 (6%)	19	46
4	D	168/189 (89%)	155 (92%)	13 (8%)	12	36
4	H	166/189 (88%)	152 (92%)	14 (8%)	10	33
All	All	1287/1486 (87%)	1184 (92%)	103 (8%)	11	35

5 of 103 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	87	THR
2	F	23	GLN
4	H	130	VAL
1	E	110	VAL
1	E	146	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 19 such sidechains are listed below:

Mol	Chain	Res	Type
2	F	69	GLN
4	H	81	HIS
4	H	157	GLN
4	H	6	HIS
3	C	101	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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
3	G	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	G	85:GLU	C	86:ALA	N	3.12

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	197/206 (95%)	-0.11	2 (1%) 79 62	22, 40, 83, 109	0
1	E	188/206 (91%)	0.93	23 (12%) 8 7	62, 99, 133, 142	0
2	B	238/241 (98%)	-0.20	3 (1%) 75 56	20, 38, 70, 107	0
2	F	229/241 (95%)	0.76	23 (10%) 12 10	60, 92, 123, 153	0
3	C	179/182 (98%)	-0.25	2 (1%) 78 60	23, 41, 72, 95	0
3	G	179/182 (98%)	0.35	6 (3%) 48 32	53, 79, 113, 132	0
4	D	199/217 (91%)	-0.28	0 100 100	27, 44, 71, 100	0
4	H	199/217 (91%)	0.27	5 (2%) 58 39	54, 73, 96, 114	0
All	All	1608/1692 (95%)	0.18	64 (3%) 42 28	20, 65, 113, 153	0

The worst 5 of 64 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	153	ASP	5.0
1	E	190	ASN	5.0
1	E	197	ASP	4.9
2	F	225	LYS	4.7
1	E	145	ASN	4.5

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.