



wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 4, 2016 – 07:48 PM EDT

PDB ID : 5J6G
Title : Recognition of the MHC class Ib molecule H2-Q10 by the natural killer cell receptor Ly49C
Authors : Berry, R.; Rossjohn, J.
Deposited on : 2016-04-04
Resolution : 3.30 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027939
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027939

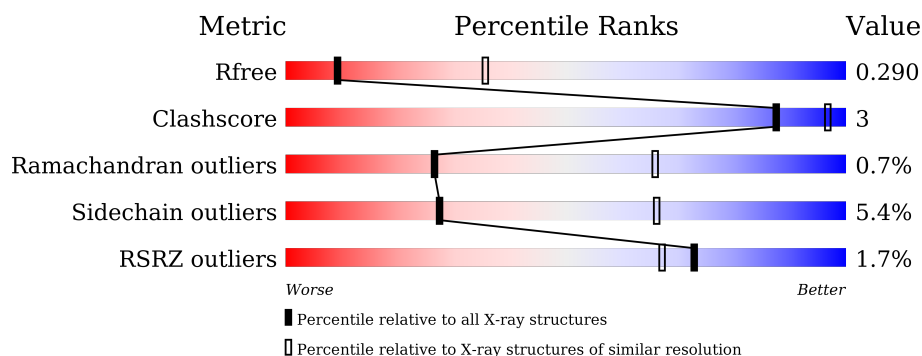
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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}	91344	2060 (3.40-3.20)
Clashscore	102246	1058 (3.38-3.22)
Ramachandran outliers	100387	1038 (3.38-3.22)
Sidechain outliers	100360	1037 (3.38-3.22)
RSRZ outliers	91569	2070 (3.40-3.20)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	300	<div> <div>2%</div> <div>80% 10% 9%</div> </div>
1	C	300	<div> <div>%</div> <div>81% 11% 8%</div> </div>
2	B	100	<div> <div>4%</div> <div>89% 10% .</div> </div>
2	D	100	<div> <div>4%</div> <div>85% 14% .</div> </div>
3	E	8	<div> <div>100%</div> </div>
3	F	8	<div> <div>100%</div> </div>

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Mol	Chain	Length	Quality of chain
4	G	132	 82%10%8%
4	H	132	 79%14%8%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7801 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 H-2 class I histocompatibility antigen, Q10 alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	272	Total	C	N	O	S	0	0	0
			2130	1361	366	394	9			
1	C	276	Total	C	N	O	S	0	0	0
			2154	1376	371	398	9			

There are 88 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	initiating methionine	UNP P01898
A	257	TYR	-	expression tag	UNP P01898
A	258	THR	-	expression tag	UNP P01898
A	259	CYS	-	expression tag	UNP P01898
A	260	HIS	-	expression tag	UNP P01898
A	261	VAL	-	expression tag	UNP P01898
A	262	TYR	-	expression tag	UNP P01898
A	263	HIS	-	expression tag	UNP P01898
A	264	GLU	-	expression tag	UNP P01898
A	265	GLY	-	expression tag	UNP P01898
A	266	LEU	-	expression tag	UNP P01898
A	267	PRO	-	expression tag	UNP P01898
A	268	GLU	-	expression tag	UNP P01898
A	269	PRO	-	expression tag	UNP P01898
A	270	LEU	-	expression tag	UNP P01898
A	271	THR	-	expression tag	UNP P01898
A	272	LEU	-	expression tag	UNP P01898
A	273	ARG	-	expression tag	UNP P01898
A	274	TRP	-	expression tag	UNP P01898
A	275	GLU	-	expression tag	UNP P01898
A	276	PRO	-	expression tag	UNP P01898
A	277	PRO	-	expression tag	UNP P01898
A	278	PRO	-	expression tag	UNP P01898
A	279	SER	-	expression tag	UNP P01898
A	280	ALA	-	expression tag	UNP P01898

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Chain	Residue	Modelled	Actual	Comment	Reference
A	281	SER	-	expression tag	UNP P01898
A	282	GLY	-	expression tag	UNP P01898
A	283	SER	-	expression tag	UNP P01898
A	284	GLY	-	expression tag	UNP P01898
A	285	LEU	-	expression tag	UNP P01898
A	286	HIS	-	expression tag	UNP P01898
A	287	HIS	-	expression tag	UNP P01898
A	288	ILE	-	expression tag	UNP P01898
A	289	LEU	-	expression tag	UNP P01898
A	290	ASP	-	expression tag	UNP P01898
A	291	ALA	-	expression tag	UNP P01898
A	292	GLN	-	expression tag	UNP P01898
A	293	LYS	-	expression tag	UNP P01898
A	294	MET	-	expression tag	UNP P01898
A	295	VAL	-	expression tag	UNP P01898
A	296	TRP	-	expression tag	UNP P01898
A	297	ASN	-	expression tag	UNP P01898
A	298	HIS	-	expression tag	UNP P01898
A	299	ARG	-	expression tag	UNP P01898
C	0	MET	-	initiating methionine	UNP P01898
C	257	TYR	-	expression tag	UNP P01898
C	258	THR	-	expression tag	UNP P01898
C	259	CYS	-	expression tag	UNP P01898
C	260	HIS	-	expression tag	UNP P01898
C	261	VAL	-	expression tag	UNP P01898
C	262	TYR	-	expression tag	UNP P01898
C	263	HIS	-	expression tag	UNP P01898
C	264	GLU	-	expression tag	UNP P01898
C	265	GLY	-	expression tag	UNP P01898
C	266	LEU	-	expression tag	UNP P01898
C	267	PRO	-	expression tag	UNP P01898
C	268	GLU	-	expression tag	UNP P01898
C	269	PRO	-	expression tag	UNP P01898
C	270	LEU	-	expression tag	UNP P01898
C	271	THR	-	expression tag	UNP P01898
C	272	LEU	-	expression tag	UNP P01898
C	273	ARG	-	expression tag	UNP P01898
C	274	TRP	-	expression tag	UNP P01898
C	275	GLU	-	expression tag	UNP P01898
C	276	PRO	-	expression tag	UNP P01898
C	277	PRO	-	expression tag	UNP P01898
C	278	PRO	-	expression tag	UNP P01898

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Chain	Residue	Modelled	Actual	Comment	Reference
C	279	SER	-	expression tag	UNP P01898
C	280	ALA	-	expression tag	UNP P01898
C	281	SER	-	expression tag	UNP P01898
C	282	GLY	-	expression tag	UNP P01898
C	283	SER	-	expression tag	UNP P01898
C	284	GLY	-	expression tag	UNP P01898
C	285	LEU	-	expression tag	UNP P01898
C	286	HIS	-	expression tag	UNP P01898
C	287	HIS	-	expression tag	UNP P01898
C	288	ILE	-	expression tag	UNP P01898
C	289	LEU	-	expression tag	UNP P01898
C	290	ASP	-	expression tag	UNP P01898
C	291	ALA	-	expression tag	UNP P01898
C	292	GLN	-	expression tag	UNP P01898
C	293	LYS	-	expression tag	UNP P01898
C	294	MET	-	expression tag	UNP P01898
C	295	VAL	-	expression tag	UNP P01898
C	296	TRP	-	expression tag	UNP P01898
C	297	ASN	-	expression tag	UNP P01898
C	298	HIS	-	expression tag	UNP P01898
C	299	ARG	-	expression tag	UNP P01898

- 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
			734	469	121	137	7			
2	D	99	Total	C	N	O	S	0	0	0
			749	479	125	138	7			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	MET	-	initiating methionine	UNP P01887
D	0	MET	-	initiating methionine	UNP P01887

- Molecule 3 is a protein called VAL-GLY-ILE-THR-ASN-VAL-ASP-LEU.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	E	8	Total	C	N	O	0	0	0
			57	36	9	12			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	F	8	Total	C	N	O	0	0	0
			57	36	9	12			

- Molecule 4 is a protein called Killer cell lectin-like receptor 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	G	122	Total	C	N	O	S	0	0	0
			963	631	153	168	11			
4	H	122	Total	C	N	O	S	0	0	0
			957	623	154	170	10			

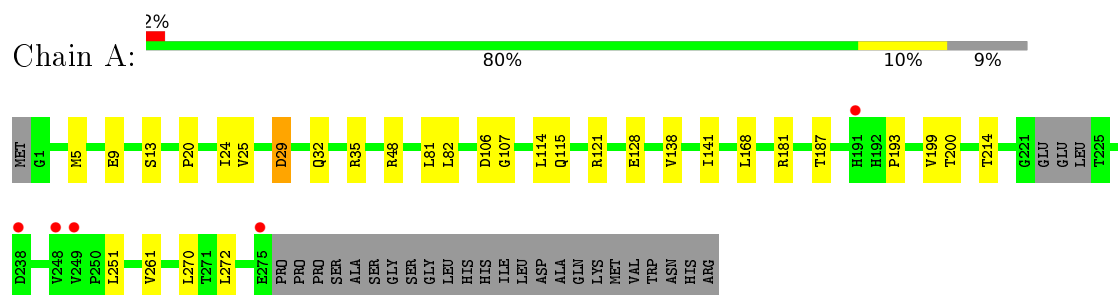
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	135	MET	-	initiating methionine	UNP Q64329
H	135	MET	-	initiating methionine	UNP Q64329

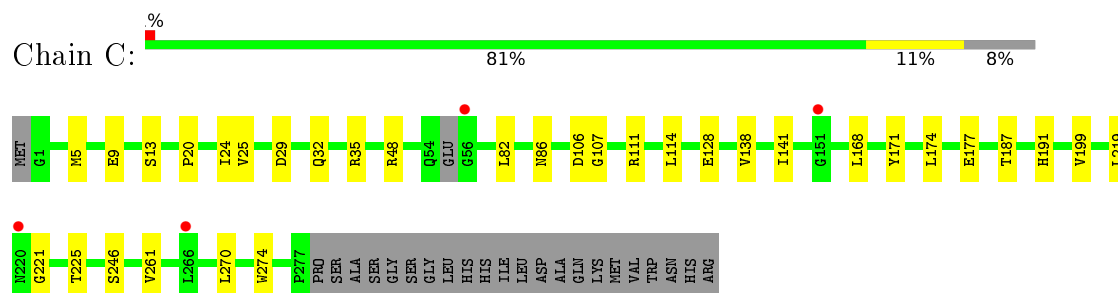
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

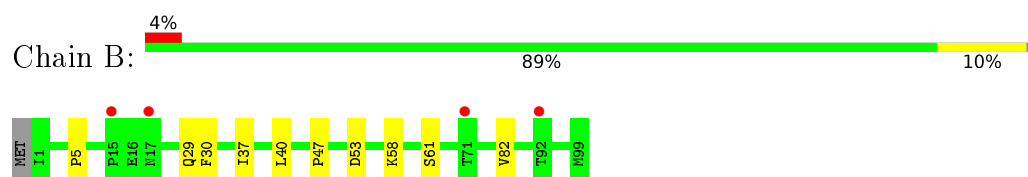
- Molecule 1: H-2 class I histocompatibility antigen, Q10 alpha chain



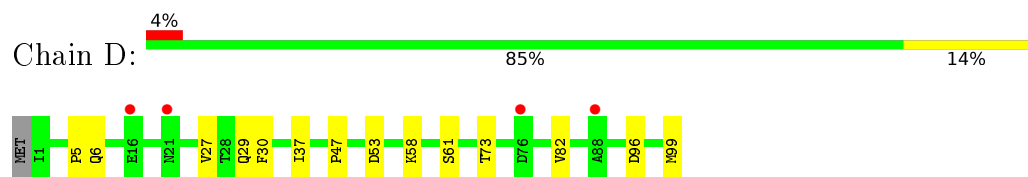
- Molecule 1: H-2 class I histocompatibility antigen, Q10 alpha chain



- Molecule 2: Beta-2-microglobulin



- Molecule 2: Beta-2-microglobulin



- Molecule 3: VAL-GLY-ILE-THR-ASN-VAL-ASP-LEU




There are no outlier residues recorded for this chain.

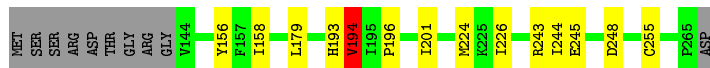
- Molecule 3: VAL-GLY-ILE-THR-ASN-VAL-ASP-LEU

Chain F:  100%


There are no outlier residues recorded for this chain.

- Molecule 4: Killer cell lectin-like receptor 3

Chain G:  82% 10% • 8%



- Molecule 4: Killer cell lectin-like receptor 3

Chain H:  79% 14% 8%



4 Data and refinement statistics

Property	Value	Source
Space group	I 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	101.01Å 57.80Å 210.70Å 90.00° 96.15° 90.00°	Depositor
Resolution (Å)	46.16 – 3.30 46.16 – 3.30	Depositor EDS
% Data completeness (in resolution range)	99.9 (46.16-3.30) 99.9 (46.16-3.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.05 (at 3.32Å)	Xtriage
Refinement program	BUSTER 2.10.0	Depositor
R, R_{free}	0.221 , 0.253 0.254 , 0.290	Depositor DCC
R_{free} test set	948 reflections (5.11%)	DCC
Wilson B-factor (Å ²)	47.1	Xtriage
Anisotropy	0.224	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 48.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.82	EDS
Total number of atoms	7801	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.12% 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	0.36	0/2194	0.51	0/2999
1	C	0.36	0/2220	0.53	0/3036
2	B	0.37	0/758	0.51	0/1043
2	D	0.36	0/775	0.50	0/1064
3	E	0.37	0/56	0.59	0/76
3	F	0.37	0/56	0.58	0/76
4	G	0.38	0/994	0.57	0/1353
4	H	0.40	0/988	0.54	0/1348
All	All	0.37	0/8041	0.53	0/10995

There are no bond length outliers.

There are no bond angle outliers.

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	2130	0	1942	11	0
1	C	2154	0	1960	12	0
2	B	734	0	630	5	0
2	D	749	0	652	7	0
3	E	57	0	62	0	0
3	F	57	0	62	0	0
4	G	963	0	866	5	0
4	H	957	0	839	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	7801	0	7013	39	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 3.

The worst 5 of 39 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:C:5:MET:HB2	1:C:168:LEU:HD13	1.85	0.58
2:B:29:GLN:HA	2:B:61:SER:HB2	1.85	0.57
1:A:193:PRO:HA	1:A:199:VAL:HG12	1.87	0.57
2:D:29:GLN:HA	2:D:61:SER:HB2	1.86	0.56
1:A:5:MET:HB2	1:A:168:LEU:HD13	1.89	0.54

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	268/300 (89%)	252 (94%)	15 (6%)	1 (0%)	39	76
1	C	272/300 (91%)	256 (94%)	14 (5%)	2 (1%)	26	66
2	B	97/100 (97%)	92 (95%)	4 (4%)	1 (1%)	19	58
2	D	97/100 (97%)	92 (95%)	4 (4%)	1 (1%)	19	58
3	E	6/8 (75%)	6 (100%)	0	0	100	100
3	F	6/8 (75%)	6 (100%)	0	0	100	100
4	G	120/132 (91%)	109 (91%)	10 (8%)	1 (1%)	24	62
4	H	120/132 (91%)	111 (92%)	8 (7%)	1 (1%)	24	62
All	All	986/1080 (91%)	924 (94%)	55 (6%)	7 (1%)	26	66

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	29	ASP
2	B	47	PRO
1	C	29	ASP
1	C	221	GLY
2	D	47	PRO

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	206/255 (81%)	194 (94%)	12 (6%)	25	64
1	C	209/255 (82%)	199 (95%)	10 (5%)	31	70
2	B	72/94 (77%)	71 (99%)	1 (1%)	74	88
2	D	75/94 (80%)	73 (97%)	2 (3%)	52	81
3	E	7/7 (100%)	7 (100%)	0	100	100
3	F	7/7 (100%)	7 (100%)	0	100	100
4	G	96/122 (79%)	89 (93%)	7 (7%)	17	53
4	H	94/122 (77%)	85 (90%)	9 (10%)	10	38
All	All	766/956 (80%)	725 (95%)	41 (5%)	27	66

5 of 41 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	199	VAL
1	C	270	LEU
4	H	223	ASP
1	C	219	LEU
1	C	225	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	260	HIS
1	C	115	GLN
1	C	32	GLN
1	A	75	HIS
1	C	75	HIS

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 carbohydrates 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	272/300 (90%)	0.20	5 (1%) 71 65	20, 44, 89, 138	0
1	C	276/300 (92%)	0.20	4 (1%) 78 73	26, 50, 78, 113	0
2	B	99/100 (99%)	0.25	4 (4%) 42 34	23, 49, 63, 71	0
2	D	99/100 (99%)	0.33	4 (4%) 42 34	30, 56, 72, 78	0
3	E	8/8 (100%)	0.13	0 100 100	31, 34, 38, 52	0
3	F	8/8 (100%)	-0.14	0 100 100	29, 32, 38, 60	0
4	G	122/132 (92%)	-0.11	0 100 100	17, 38, 58, 71	0
4	H	122/132 (92%)	-0.04	0 100 100	21, 41, 64, 110	0
All	All	1006/1080 (93%)	0.15	17 (1%) 73 67	17, 47, 77, 138	0

The worst 5 of 17 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	21	ASN	4.1
1	C	220	ASN	3.4
2	D	76	ASP	2.8
1	A	191	HIS	2.6
1	C	151	GLY	2.5

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 carbohydrates 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.