



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 4, 2025 – 05:17 PM JST

PDB ID : 9J4T / pdb\_00009j4t  
Title : Structural basis for recognition of SARS-CoV-2 conserved nucleocapside epitopes by dominant T cell receptors  
Authors : Yuan, P.; Wu, D.C.  
Deposited on : 2024-08-10  
Resolution : 2.04 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](mailto: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>.

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

MolProbity	:	4-5-2 with Phenix2.0rc1
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.45.1

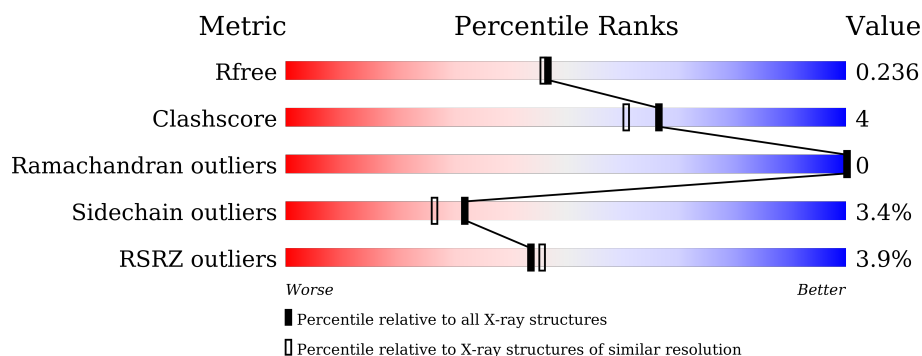
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.04 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))
$R_{free}$	164625	2096 (2.04-2.04)
Clashscore	180529	2229 (2.04-2.04)
Ramachandran outliers	177936	2217 (2.04-2.04)
Sidechain outliers	177891	2217 (2.04-2.04)
RSRZ outliers	164620	2096 (2.04-2.04)

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  $\geq 3$ , 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	<div> <div>7%</div> <div>87%</div> <div>11%</div> <div>..</div> </div>
2	B	100	<div> <div>7%</div> <div>83%</div> <div>16%</div> <div>.</div> </div>
3	C	9	<div> <div>89%</div> <div>11%</div> </div>
4	D	205	<div> <div>3%</div> <div>83%</div> <div>9%</div> <div>6%</div> </div>
5	E	244	<div> <div>89%</div> <div>11%</div> </div>

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 7308 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 HLA class I histocompatibility antigen, B alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	273	Total	C	N	O	S	0	0	0
			2238	1389	410	433	6			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	initiating methionine	UNP P01889

- 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
			833	530	140	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 Nucleoprotein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	9	Total	C	N	O	0	0	0
			94	67	13	14			

- Molecule 4 is a protein called SPR epitope specific TCR CLB1 ALPHA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	192	Total	C	N	O	S	0	0	0
			1481	915	256	302	8			

- Molecule 5 is a protein called SPR epitope specific TCR CLB1 BETA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	243	Total 1940	C 1229	N 334	O 367	S 10	0	0	0

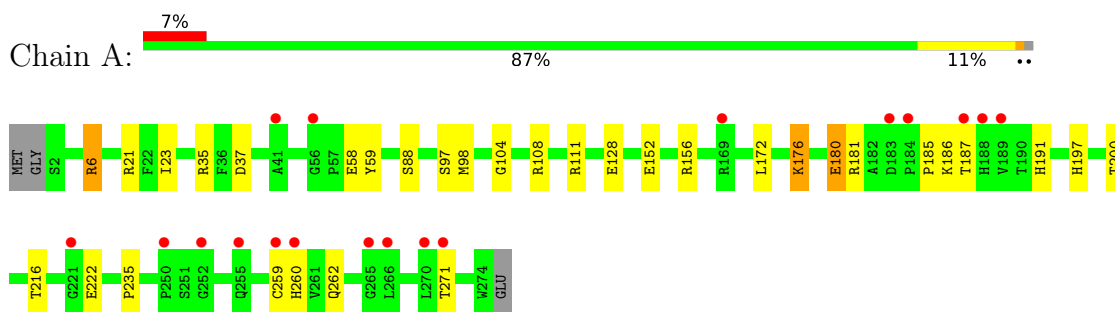
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	223	Total 223	O 223	0	0
6	B	64	Total 64	O 64	0	0
6	C	8	Total 8	O 8	0	0
6	D	193	Total 193	O 193	0	0
6	E	234	Total 234	O 234	0	0

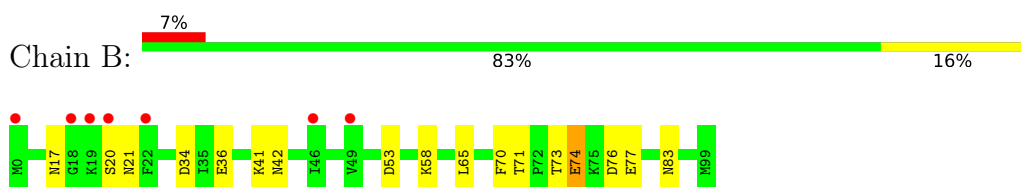
### 3 Residue-property plots [i](#)

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.

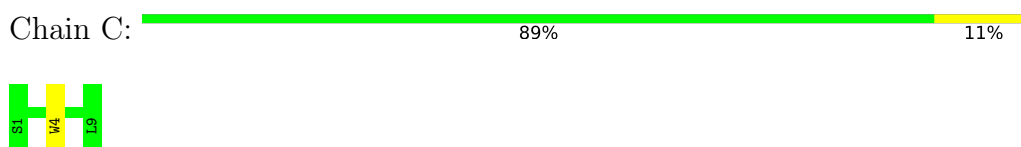
- Molecule 1: HLA class I histocompatibility antigen, B alpha chain



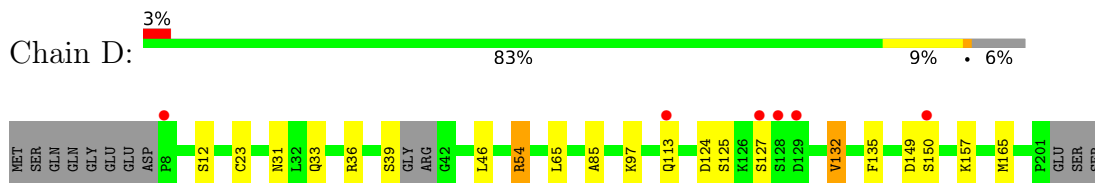
- Molecule 2: Beta-2-microglobulin



- Molecule 3: Nucleoprotein

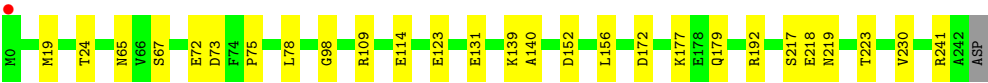


- Molecule 4: SPR epitope specific TCR CLB1 ALPHA



- Molecule 5: SPR epitope specific TCR CLB1 BETA





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	58.10Å 102.72Å 160.15Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.90 – 2.04 48.90 – 2.04	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.90-2.04) 100.0 (48.90-2.04)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.64 (at 2.05Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, $R_{free}$	0.187 , 0.232 0.197 , 0.236	Depositor DCC
$R_{free}$ test set	3093 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	25.4	Xtriage
Anisotropy	0.025	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 42.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	7308	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.41% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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	1.14	4/2300 (0.2%)	1.05	4/3126 (0.1%)
2	B	1.03	0/856	1.01	0/1158
3	C	1.04	0/100	0.94	0/135
4	D	1.16	3/1507 (0.2%)	1.11	2/2041 (0.1%)
5	E	1.14	2/1994 (0.1%)	1.06	6/2715 (0.2%)
All	All	1.13	9/6757 (0.1%)	1.06	12/9175 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	97	SER	C-O	7.34	1.32	1.23
4	D	85	ALA	CA-C	-5.92	1.45	1.52
1	A	197	HIS	CA-C	5.38	1.59	1.52
4	D	23	CYS	CA-C	-5.36	1.46	1.52
1	A	6	ARG	CA-C	-5.34	1.45	1.52
5	E	140	ALA	N-CA	-5.27	1.40	1.46
5	E	177	LYS	CA-C	-5.09	1.46	1.52
1	A	172	LEU	C-O	5.08	1.30	1.24
4	D	135	PHE	CA-C	-5.03	1.46	1.52

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	19	MET	CG-SD-CE	-6.96	85.59	100.90
1	A	59	TYR	N-CA-C	-6.42	103.90	111.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	104	GLY	CA-C-N	6.26	126.46	119.32
1	A	104	GLY	C-N-CA	6.26	126.46	119.32
1	A	176	LYS	CB-CA-C	-6.21	108.79	117.23
5	E	172	ASP	CA-C-N	5.55	125.21	119.05
5	E	172	ASP	C-N-CA	5.55	125.21	119.05
5	E	19	MET	N-CA-CB	-5.41	103.17	111.56
5	E	65	ASN	CB-CA-C	-5.41	98.17	110.07
4	D	132	VAL	N-CA-CB	-5.33	101.96	111.92
5	E	230	VAL	CB-CA-C	-5.16	105.91	111.59
4	D	54	ARG	N-CA-C	-5.10	107.61	113.88

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	185	PRO	Peptide

## 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	2238	0	2075	15	0
2	B	833	0	792	11	0
3	C	94	0	84	1	0
4	D	1481	0	1420	11	1
5	E	1940	0	1854	13	1
6	A	223	0	0	2	0
6	B	64	0	0	1	0
6	C	8	0	0	0	0
6	D	193	0	0	2	0
6	E	234	0	0	4	0
All	All	7308	0	6225	46	1

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 (46) 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)
4:D:165:MET:HE1	5:E:139:LYS:HE3	1.54	0.86
5:E:24:THR:HG22	5:E:73:ASP:OD1	1.74	0.86
4:D:39:SER:HB3	6:D:463:HOH:O	1.75	0.85
1:A:259:CYS:SG	6:A:303:HOH:O	2.39	0.81
4:D:150:SER:O	6:D:301:HOH:O	2.08	0.71
4:D:165:MET:CE	5:E:139:LYS:HE3	2.22	0.69
1:A:216:THR:C	6:A:303:HOH:O	2.40	0.64
5:E:218:GLU:HA	6:E:315:HOH:O	2.00	0.62
2:B:36:GLU:OE1	2:B:83:ASN:HB2	2.02	0.59
1:A:176:LYS:O	1:A:180:GLU:HG3	2.02	0.59
2:B:21:ASN:N	2:B:70:PHE:O	2.35	0.58
5:E:179:GLN:NE2	5:E:179:GLN:HA	2.20	0.56
1:A:152:GLU:O	1:A:156:ARG:HG2	2.06	0.55
1:A:6:ARG:HD2	1:A:98:MET:SD	2.46	0.55
4:D:31:ASN:HD21	4:D:33:GLN:HE21	1.54	0.54
2:B:73:THR:OG1	2:B:76:ASP:OD2	2.26	0.51
1:A:260:HIS:CE1	1:A:271:THR:OG1	2.64	0.50
5:E:152:ASP:CG	5:E:152:ASP:O	2.54	0.50
1:A:21:ARG:NH2	1:A:37:ASP:OD2	2.42	0.49
4:D:54:ARG:HD3	4:D:65:LEU:O	2.13	0.49
5:E:218:GLU:HG2	6:E:486:HOH:O	2.12	0.49
4:D:31:ASN:ND2	4:D:33:GLN:HE21	2.11	0.49
5:E:67:SER:O	5:E:75:PRO:HD2	2.13	0.48
2:B:17:ASN:HD21	2:B:74:GLU:HG2	1.79	0.46
1:A:235:PRO:HG2	2:B:65:LEU:HD22	1.97	0.46
4:D:149:ASP:OD1	4:D:149:ASP:C	2.58	0.46
1:A:176:LYS:O	1:A:180:GLU:CG	2.63	0.46
2:B:17:ASN:ND2	2:B:74:GLU:HG2	2.31	0.46
2:B:21:ASN:HB3	2:B:70:PHE:CE1	2.52	0.44
4:D:124:ASP:HB3	4:D:127:SER:O	2.18	0.44
4:D:149:ASP:OD1	4:D:150:SER:N	2.51	0.44
2:B:41:LYS:O	2:B:42:ASN:C	2.61	0.44
5:E:24:THR:HA	5:E:72:GLU:O	2.19	0.43
4:D:36:ARG:HB2	4:D:46:LEU:HD11	2.01	0.42
1:A:111:ARG:CZ	1:A:128:GLU:HB3	2.49	0.42
5:E:241:ARG:NH1	6:E:312:HOH:O	2.52	0.42
5:E:156:LEU:C	5:E:156:LEU:HD23	2.44	0.42
2:B:17:ASN:OD1	2:B:73:THR:HA	2.18	0.42
5:E:123:GLU:CD	6:E:305:HOH:O	2.63	0.41
1:A:35:ARG:HD3	2:B:53:ASP:OD2	2.21	0.41
1:A:58:GLU:H	1:A:58:GLU:CD	2.29	0.41
1:A:191:HIS:HA	1:A:200:THR:O	2.22	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:34:ASP:HB2	6:B:145:HOH:O	2.21	0.41
1:A:186:LYS:O	1:A:187:THR:CG2	2.69	0.40
3:C:4:TRP:CH2	5:E:98:GLY:HA2	2.56	0.40
1:A:260:HIS:CE1	1:A:271:THR:HG1	2.38	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:113:GLN:OE1	5:E:223:THR:OG1[1_455]	2.00	0.20

## 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	271/276 (98%)	261 (96%)	10 (4%)	0	100	100
2	B	98/100 (98%)	93 (95%)	5 (5%)	0	100	100
3	C	7/9 (78%)	7 (100%)	0	0	100	100
4	D	188/205 (92%)	183 (97%)	5 (3%)	0	100	100
5	E	241/244 (99%)	237 (98%)	4 (2%)	0	100	100
All	All	805/834 (96%)	781 (97%)	24 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

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	231/234 (99%)	224 (97%)	7 (3%)	36	31
2	B	94/95 (99%)	89 (95%)	5 (5%)	19	12
3	C	9/9 (100%)	9 (100%)	0	100	100
4	D	170/183 (93%)	165 (97%)	5 (3%)	37	32
5	E	210/211 (100%)	203 (97%)	7 (3%)	33	27
All	All	714/732 (98%)	690 (97%)	24 (3%)	32	26

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	ILE
1	A	88	SER
1	A	108	ARG
1	A	180	GLU
1	A	181	ARG
1	A	222	GLU
1	A	262	GLN
2	B	20	SER
2	B	58	LYS
2	B	71	THR
2	B	74	GLU
2	B	77	GLU
4	D	12	SER
4	D	97	LYS
4	D	125	SER
4	D	132	VAL
4	D	157	LYS
5	E	78	LEU
5	E	109	ARG
5	E	114	GLU
5	E	131	GLU
5	E	192	ARG
5	E	217	SER
5	E	219	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	141	GLN
1	A	144	GLN
1	A	192	HIS
1	A	260	HIS
1	A	262	GLN
2	B	13	HIS
4	D	14	GLN
4	D	31	ASN
4	D	141	GLN
5	E	22	GLN
5	E	166	HIS
5	E	179	GLN
5	E	219	ASN

### 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 ⓘ

### 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	273/276 (98%)	0.29	18 (6%) 26 27	12, 34, 63, 81	0
2	B	100/100 (100%)	0.49	7 (7%) 24 26	15, 38, 64, 73	0
3	C	9/9 (100%)	-0.65	0 100 100	16, 18, 20, 25	0
4	D	192/205 (93%)	-0.05	6 (3%) 51 53	15, 28, 55, 75	0
5	E	243/244 (99%)	-0.29	1 (0%) 89 90	14, 23, 44, 65	0
All	All	817/834 (97%)	0.05	32 (3%) 44 46	12, 28, 59, 81	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	265	GLY	3.0
1	A	266	LEU	3.0
1	A	188	HIS	2.6
2	B	0	MET	2.6
1	A	271	THR	2.6
2	B	18	GLY	2.5
1	A	189	VAL	2.5
1	A	187	THR	2.5
1	A	270	LEU	2.4
2	B	19	LYS	2.4
1	A	255	GLN	2.4
4	D	128	SER	2.4
4	D	8	PRO	2.3
1	A	260	HIS	2.3
1	A	169	ARG	2.3
4	D	113	GLN	2.3
5	E	0	MET	2.2
1	A	259	CYS	2.2
4	D	129	ASP	2.2
1	A	221	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
4	D	127	SER	2.2
1	A	184	PRO	2.2
1	A	56	GLY	2.2
2	B	49	VAL	2.2
1	A	252	GLY	2.2
2	B	22	PHE	2.1
2	B	46	ILE	2.1
4	D	150	SER	2.1
1	A	250	PRO	2.0
2	B	20	SER	2.0
1	A	41	ALA	2.0
1	A	183	ASP	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.