



# Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 05:44 pm BST

PDB ID : 6PX6  
Title : HLA-TCR complex  
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Deposited on : 2019-07-24  
Resolution : 3.00 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.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

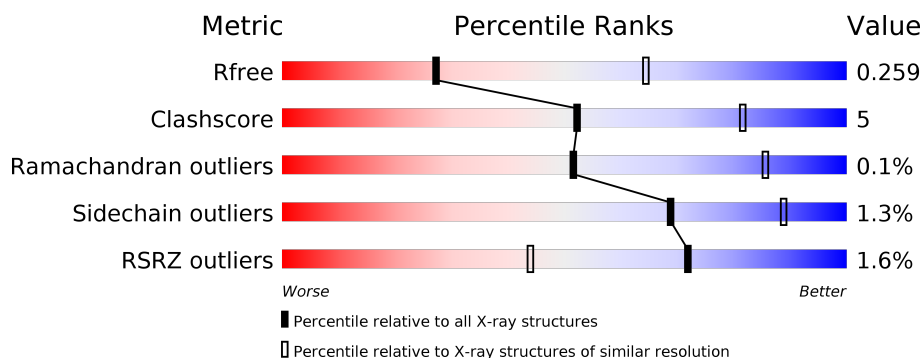
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 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))
$R_{free}$	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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 on 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	254	
2	B	261	
3	C	12	
4	D	217	
5	E	256	

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 6291 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 II histocompatibility antigen DQ alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	179	Total	C	N	O	S	0	0	0
			1436	930	231	273	2			

- Molecule 2 is a protein called HLA class II histocompatibility antigen DQ beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	178	Total	C	N	O	S	0	0	0
			1432	909	250	266	7			

- Molecule 3 is a protein called DQ2.2-glut-L1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	12	Total	C	N	O	0	0	0
			91	58	14	19			

- Molecule 4 is a protein called T-cell receptor, T1005.2.56, alpha chain, Human nkt tcr alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	190	Total	C	N	O	S	0	0	0
			1427	882	242	295	8			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	202	LYS	-	expression tag	UNP K7N5M3
D	203	LEU	-	expression tag	UNP K7N5M3
D	204	ALA	-	expression tag	UNP K7N5M3
D	205	ALA	-	expression tag	UNP K7N5M3
D	206	ALA	-	expression tag	UNP K7N5M3
D	207	LEU	-	expression tag	UNP K7N5M3
D	208	GLU	-	expression tag	UNP K7N5M3

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Chain	Residue	Modelled	Actual	Comment	Reference
D	209	HIS	-	expression tag	UNP K7N5M3
D	210	HIS	-	expression tag	UNP K7N5M3
D	211	HIS	-	expression tag	UNP K7N5M3
D	212	HIS	-	expression tag	UNP K7N5M3
D	213	HIS	-	expression tag	UNP K7N5M3

- Molecule 5 is a protein called T-cell receptor, T1005.2.56, beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	241	Total	C	N	O	S	0	0	0
			1880	1183	328	364	5			

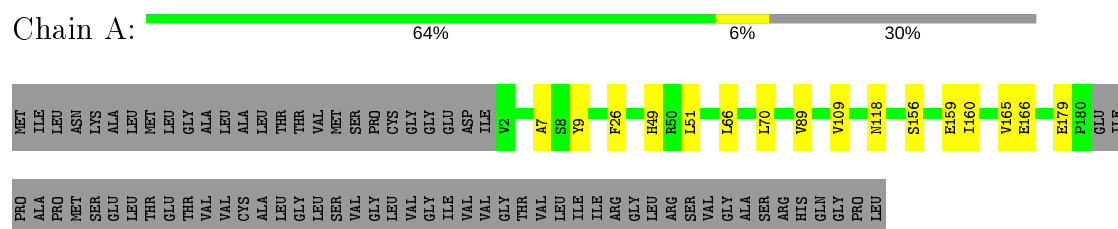
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	10	Total	O	0	0
			10	10		
6	B	3	Total	O	0	0
			3	3		
6	C	1	Total	O	0	0
			1	1		
6	D	5	Total	O	0	0
			5	5		
6	E	6	Total	O	0	0
			6	6		

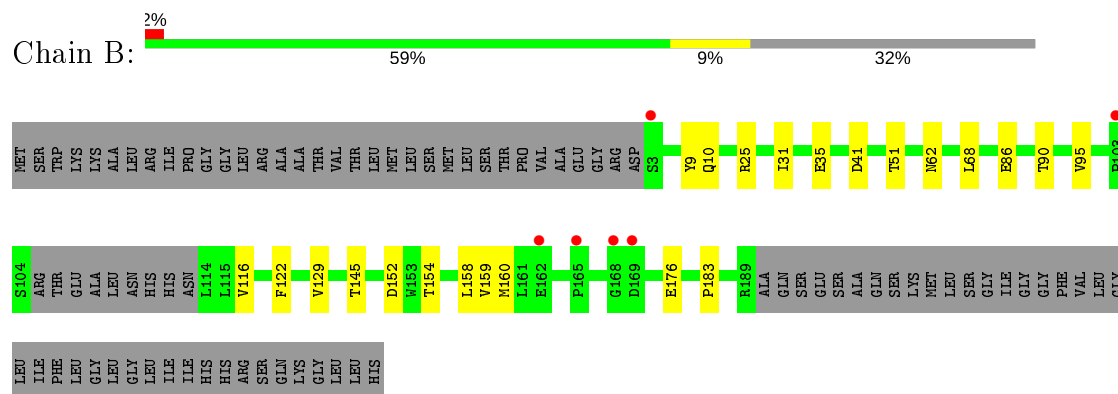
### 3 Residue-property plots [i](#)

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

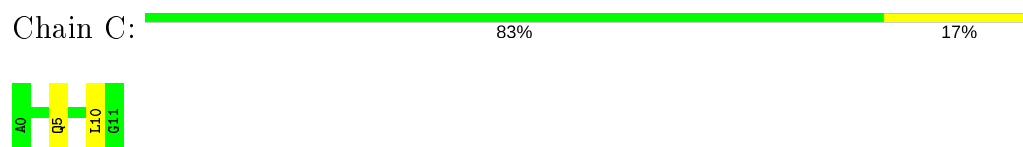
- Molecule 1: HLA class II histocompatibility antigen DQ alpha chain



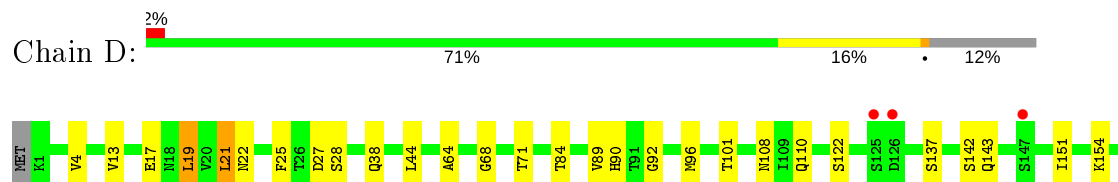
- Molecule 2: HLA class II histocompatibility antigen DQ beta chain

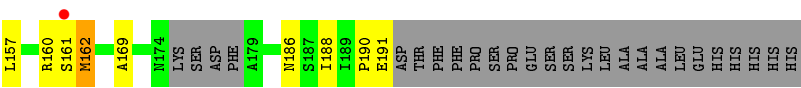


- Molecule 3: DQ2.2-glut-L1

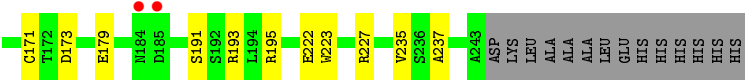
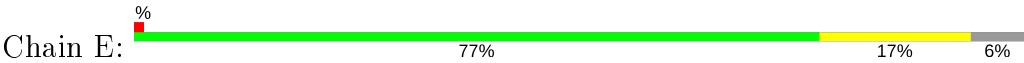


- Molecule 4: T-cell receptor, T1005.2.56, alpha chain, Human nkt tcr alpha chain





● Molecule 5: T-cell receptor, T1005.2.56, beta chain



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	72.53 Å 99.42 Å 72.56 Å 90.00° 118.26° 90.00°	Depositor
Resolution (Å)	39.24 – 3.00 39.24 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.9 (39.24-3.00) 94.1 (39.24-3.00)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.22 (at 3.01 Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, $R_{free}$	0.205 , 0.257 0.205 , 0.259	Depositor DCC
$R_{free}$ test set	950 reflections (5.20%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	37.2	Xtriage
Anisotropy	0.319	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 39.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.008 for -h-l,k,h 0.008 for l,k,-h-l 0.029 for h,-k,-h-l 0.035 for -h-l,-k,l 0.032 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	6291	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.53% 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

### 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	0.26	0/1480	0.43	0/2023
2	B	0.24	0/1465	0.44	0/1995
3	C	0.27	0/93	0.41	0/126
4	D	0.26	0/1450	0.52	0/1972
5	E	0.25	0/1932	0.45	0/2636
All	All	0.25	0/6420	0.46	0/8752

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

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	1436	0	1374	11	0
2	B	1432	0	1381	14	0
3	C	91	0	86	2	0
4	D	1427	0	1354	21	0
5	E	1880	0	1762	27	0
6	A	10	0	0	0	0
6	B	3	0	0	0	0
6	C	1	0	0	0	0
6	D	5	0	0	0	0
6	E	6	0	0	0	0
All	All	6291	0	5957	67	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.

All (67) 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:49:HIS:HB2	1:A:51:LEU:HD12	1.71	0.73
5:E:14:GLU:HG2	5:E:15:LYS:H	1.56	0.69
4:D:142:SER:HB2	4:D:186:ASN:HB3	1.73	0.69
2:B:10:GLN:HB2	2:B:31:ILE:HB	1.79	0.65
2:B:176:GLU:HG2	2:B:183:PRO:HB3	1.78	0.65
4:D:13:VAL:HG21	4:D:17:GLU:HG2	1.79	0.63
4:D:90:HIS:CD2	5:E:100:THR:HG22	2.34	0.63
5:E:15:LYS:HD3	5:E:115:GLU:HG3	1.80	0.63
5:E:171:CYS:HB3	5:E:193:ARG:HB2	1.80	0.62
2:B:35:GLU:OE2	2:B:51:THR:HG21	2.02	0.59
4:D:188:ILE:HG22	4:D:190:PRO:HD2	1.84	0.59
2:B:116:VAL:HG12	2:B:160:MET:HG2	1.85	0.58
4:D:137:SER:O	4:D:154:LYS:NZ	2.36	0.58
5:E:34:TRP:HB2	5:E:47:ILE:HG22	1.85	0.58
1:A:89:VAL:HG22	1:A:109:VAL:HG12	1.84	0.58
4:D:4:VAL:HG12	4:D:25:PHE:HB3	1.85	0.58
1:A:70:LEU:HD13	2:B:9:TYR:HB2	1.86	0.56
2:B:145:THR:HG22	2:B:158:LEU:H	1.72	0.55
4:D:160:ARG:O	4:D:162:MET:N	2.37	0.55
5:E:125:VAL:HG12	5:E:235:VAL:HG12	1.90	0.54
2:B:62:ASN:HA	2:B:68:LEU:HD21	1.90	0.53
5:E:84:ARG:HD2	5:E:115:GLU:HB2	1.90	0.53
4:D:27:ASP:OD2	4:D:28:SER:N	2.42	0.53
1:A:7:ALA:HB2	1:A:26:PHE:HD1	1.74	0.52
1:A:118:ASN:HB2	1:A:166:GLU:HB2	1.91	0.51
2:B:152:ASP:OD1	2:B:154:THR:OG1	2.26	0.50
4:D:157:LEU:HB3	5:E:171:CYS:HB2	1.94	0.50
4:D:108:ASN:OD1	4:D:110:GLN:NE2	2.43	0.49
4:D:89:VAL:HG12	4:D:96:MET:HB3	1.94	0.49
5:E:173:ASP:OD1	5:E:193:ARG:NH1	2.39	0.49
2:B:25:ARG:NH2	2:B:41:ASP:OD2	2.44	0.48
1:A:160:ILE:HG23	1:A:179:GLU:HG2	1.96	0.48
5:E:125:VAL:HG13	5:E:237:ALA:HB2	1.96	0.48
5:E:223:TRP:NE1	5:E:227:ARG:O	2.44	0.47
1:A:66:LEU:HG	2:B:9:TYR:CD1	2.49	0.47
4:D:38:GLN:HG3	4:D:44:LEU:HD12	1.97	0.47
1:A:89:VAL:HG21	1:A:165:VAL:HG21	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:7:ALA:HB2	1:A:26:PHE:CD1	2.50	0.46
4:D:122:SER:HB3	5:E:129:GLU:HG3	1.98	0.46
5:E:123:PRO:HB3	5:E:150:PHE:HB3	1.96	0.45
2:B:86:GLU:HG3	2:B:90:THR:OG1	2.16	0.44
2:B:95:VAL:HG23	2:B:122:PHE:HA	2.00	0.44
4:D:143:GLN:HA	4:D:151:ILE:HB	1.98	0.44
4:D:19:LEU:HD23	4:D:21:LEU:HD11	2.00	0.44
5:E:11:LYS:HE3	5:E:13:THR:HG23	1.99	0.43
5:E:110:ARG:HD3	5:E:154:HIS:CD2	2.53	0.43
2:B:129:VAL:HG21	2:B:159:VAL:HG21	1.99	0.43
5:E:21:LEU:HD22	5:E:109:THR:HG21	2.01	0.43
5:E:130:PRO:HG2	5:E:141:ALA:HB1	2.01	0.43
5:E:173:ASP:OD2	5:E:191:SER:HB3	2.19	0.43
1:A:156:SER:OG	1:A:159:GLU:OE2	2.37	0.43
5:E:14:GLU:HG2	5:E:15:LYS:N	2.30	0.43
5:E:33:TYR:HB2	5:E:93:ALA:HB3	2.01	0.42
5:E:47:ILE:HD12	5:E:60:LEU:HD22	2.00	0.42
5:E:97:GLY:HA3	5:E:101:ASP:OD2	2.19	0.42
3:C:5:GLN:HE22	5:E:100:THR:HG23	1.85	0.42
4:D:22:ASN:HA	4:D:71:THR:HA	2.00	0.42
3:C:10:LEU:HD23	3:C:10:LEU:HA	1.88	0.42
4:D:90:HIS:CD2	4:D:92:GLY:H	2.38	0.42
5:E:68:VAL:HG22	5:E:70:PRO:HG3	2.01	0.42
4:D:25:PHE:CE2	4:D:68:GLY:HA2	2.56	0.41
1:A:9:TYR:OH	2:B:86:GLU:OE1	2.26	0.41
5:E:62:ASN:HB3	5:E:64:ARG:H	1.85	0.41
4:D:84:THR:HA	4:D:101:THR:O	2.20	0.41
4:D:64:ALA:HA	4:D:71:THR:O	2.21	0.40
5:E:142:THR:OG1	5:E:195:ARG:HG3	2.20	0.40
4:D:169:ALA:HA	5:E:193:ARG:HH21	1.87	0.40

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	177/254 (70%)	166 (94%)	11 (6%)	0	100	100
2	B	174/261 (67%)	163 (94%)	11 (6%)	0	100	100
3	C	10/12 (83%)	10 (100%)	0	0	100	100
4	D	186/217 (86%)	168 (90%)	17 (9%)	1 (0%)	29	68
5	E	239/256 (93%)	226 (95%)	13 (5%)	0	100	100
All	All	786/1000 (79%)	733 (93%)	52 (7%)	1 (0%)	51	85

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	161	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	163/223 (73%)	163 (100%)	0	100	100
2	B	157/229 (69%)	157 (100%)	0	100	100
3	C	10/10 (100%)	10 (100%)	0	100	100
4	D	160/190 (84%)	156 (98%)	4 (2%)	47	79
5	E	201/217 (93%)	196 (98%)	5 (2%)	47	79
All	All	691/869 (80%)	682 (99%)	9 (1%)	69	89

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	D	19	LEU
4	D	21	LEU
4	D	162	MET
4	D	191	GLU

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Mol	Chain	Res	Type
5	E	24	ASP
5	E	134	GLU
5	E	137	HIS
5	E	179	GLU
5	E	222	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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, 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	179/254 (70%)	-0.26	0 100 100	18, 33, 62, 71	0
2	B	178/261 (68%)	-0.14	6 (3%) 45 19	19, 34, 57, 74	0
3	C	12/12 (100%)	-0.53	0 100 100	21, 28, 40, 40	0
4	D	190/217 (87%)	-0.04	4 (2%) 63 34	19, 37, 71, 88	0
5	E	241/256 (94%)	-0.06	3 (1%) 79 54	18, 36, 66, 85	0
All	All	800/1000 (80%)	-0.13	13 (1%) 72 44	18, 36, 65, 88	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	D	161	SER	4.6
4	D	147	SER	4.0
5	E	185	ASP	3.2
5	E	184	ASN	3.0
2	B	169	ASP	2.8
5	E	116	ASP	2.7
2	B	165	PRO	2.5
2	B	103	PRO	2.5
2	B	3	SER	2.2
2	B	162	GLU	2.2
4	D	126	ASP	2.1
4	D	125	SER	2.1
2	B	168	GLY	2.0

### 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 [i](#)

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.