



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:52 AM GMT

PDB ID : 2V2W  
Title : T CELL CROSS-REACTIVITY AND CONFORMATIONAL CHANGES DURING TCR ENGAGEMENT  
Authors : Lee, J.K.; Stewart-Jones, G.; Dong, T.; Harlos, K.; Di Gleria, K.; Dorrell, L.; Douek, D.C.; Van Der Merwe, P.A.; Jones, E.Y.; Mcmichael, A.J.  
Deposited on : 2007-06-07  
Resolution : 1.60 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  
<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 : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
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) : trunk26865

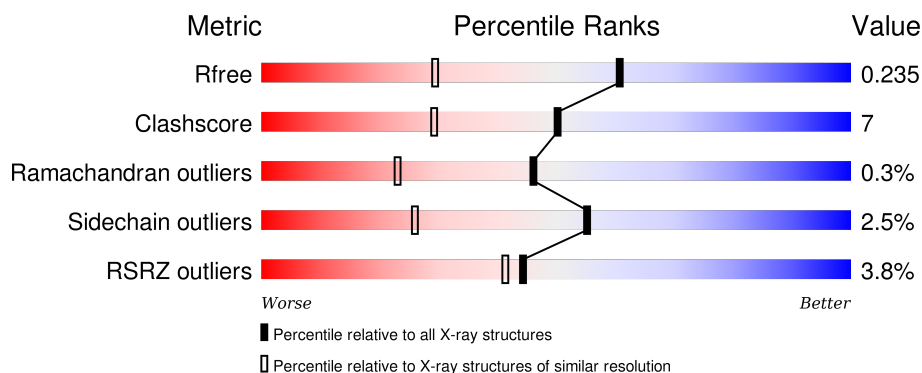
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.60 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	2475 (1.60-1.60)
Clashscore	102246	2732 (1.60-1.60)
Ramachandran outliers	100387	2654 (1.60-1.60)
Sidechain outliers	100360	2653 (1.60-1.60)
RSRZ outliers	91569	2479 (1.60-1.60)

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. 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>4%</div> <div>88%</div> <div>11%</div> </div>
1	D	276	<div> <div>4%</div> <div>87%</div> <div>12%</div> </div>
2	B	100	<div> <div>4%</div> <div>86%</div> <div>12%</div> </div>
2	E	100	<div> <div>2%</div> <div>87%</div> <div>12%</div> </div>
3	C	9	<div> <div>89%</div> <div>11%</div> </div>

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
3	F	9	 A horizontal bar chart showing the quality of chain F. The bar is divided into three segments: a red segment on the left labeled '22%', a green segment in the middle labeled '67%', and a yellow segment on the right labeled '33%'. The segments are stacked horizontally to represent the total quality score.

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 7469 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, A-2 ALPHA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	276	Total	C	N	O	S	0	0	1
			2220	1387	404	420	9			
1	D	276	Total	C	N	O	S	0	0	1
			2220	1387	404	420	9			

- 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
			817	520	140	153	4			
2	E	100	Total	C	N	O	S	0	0	0
			817	520	140	153	4			

- Molecule 3 is a protein called HIV P17.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	9	Total	C	N	O	0	0	0
			69	44	10	15			
3	F	9	Total	C	N	O	0	0	0
			69	44	10	15			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	390	Total	O	0	0
			390	390		
4	B	175	Total	O	0	0
			175	175		
4	C	18	Total	O	0	0
			18	18		
4	D	416	Total	O	0	0
			416	416		

*Continued on next page...*

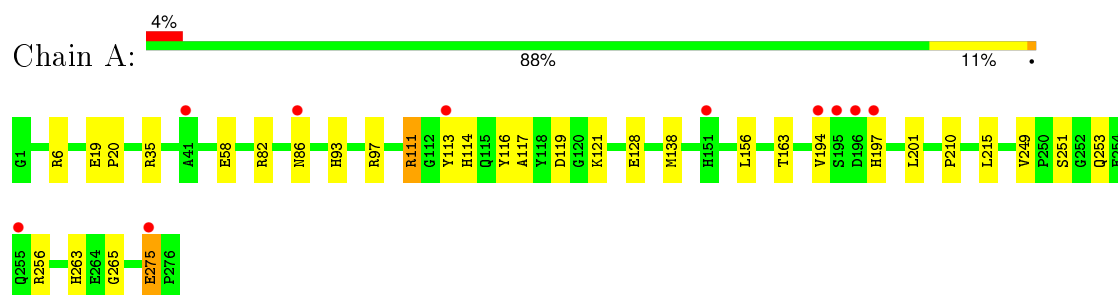
*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	240	Total	O	0	0
			240	240		
4	F	18	Total	O	0	0
			18	18		

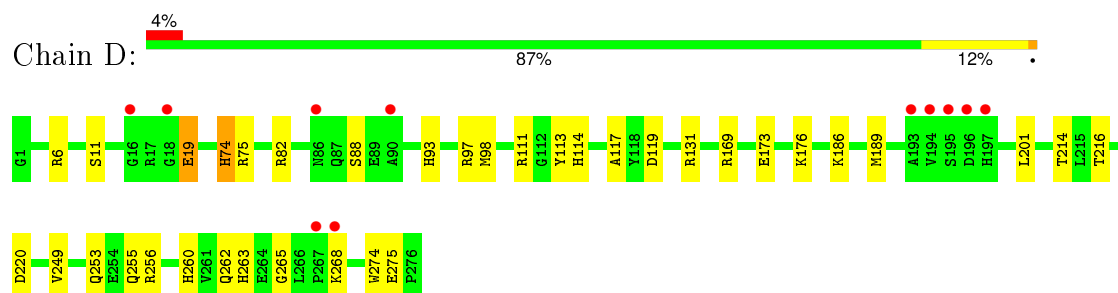
### 3 Residue-property plots [i](#)

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 ( $\text{RSRZ} > 2$ ). 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.

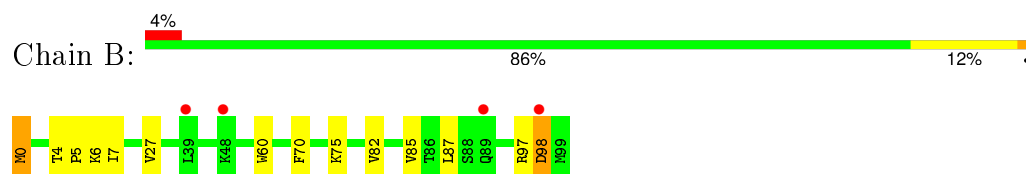
- Molecule 1: HLA CLASS I HISTOCOMPATIBILITY ANTIGEN, A-2 ALPHA CHAIN



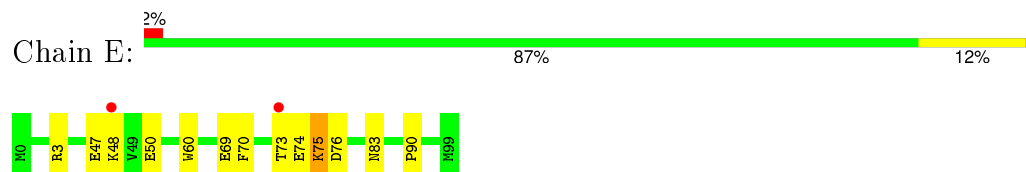
- Molecule 1: HLA CLASS I HISTOCOMPATIBILITY ANTIGEN, A-2 ALPHA CHAIN



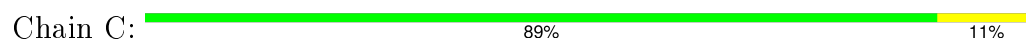
- Molecule 2: BETA-2 MICROGLOBULIN



- Molecule 2: BETA-2 MICROGLOBULIN

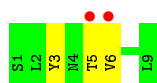


- Molecule 3: HIV P17





● Molecule 3: HIV P17



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	50.77Å 63.60Å 74.99Å 81.98° 76.26° 77.85°	Depositor
Resolution (Å)	72.55 – 1.60 23.14 – 1.60	Depositor EDS
% Data completeness (in resolution range)	86.5 (72.55-1.60) 84.9 (23.14-1.60)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.23 (at 1.60Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.199 , 0.237 0.197 , 0.235	Depositor DCC
$R_{free}$ test set	5052 reflections (5.25%)	DCC
Wilson B-factor (Å <sup>2</sup> )	19.3	Xtriage
Anisotropy	0.213	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 54.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 101201 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	7469	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.83% 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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.62	1/2284 (0.0%)	0.70	2/3100 (0.1%)
1	D	0.66	1/2284 (0.0%)	0.70	1/3100 (0.0%)
2	B	0.63	0/840	0.67	0/1135
2	E	0.70	0/840	0.69	0/1135
3	C	0.61	0/69	0.86	0/93
3	F	0.64	0/69	0.78	0/93
All	All	0.65	2/6386 (0.0%)	0.70	3/8656 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	275	GLU	C-N	-5.56	1.23	1.34
1	A	275	GLU	C-N	-5.12	1.24	1.34

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	215	LEU	CA-CB-CG	5.71	128.43	115.30
1	D	220	ASP	CB-CG-OD1	5.17	122.95	118.30
1	A	111	ARG	NE-CZ-NH1	5.14	122.87	120.30

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	2220	0	2063	23	0
1	D	2220	0	2063	34	0
2	B	817	0	776	14	0
2	E	817	0	776	13	0
3	C	69	0	72	2	0
3	F	69	0	72	8	0
4	A	390	0	0	11	0
4	B	175	0	0	6	0
4	C	18	0	0	1	0
4	D	416	0	0	10	0
4	E	240	0	0	7	0
4	F	18	0	0	0	0
All	All	7469	0	5822	84	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 7.

All (84) 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:E:73:THR:HB	4:E:2185:HOH:O	1.43	1.16
1:A:58:GLU:HG3	4:A:2117:HOH:O	1.44	1.16
2:E:47:GLU:CA	4:E:2147:HOH:O	1.98	1.10
1:D:255:GLN:HG2	4:D:2384:HOH:O	1.73	0.87
2:E:74:GLU:CA	4:E:2190:HOH:O	2.24	0.84
1:A:251:SER:HA	4:A:2369:HOH:O	1.78	0.82
1:D:263:HIS:HD2	1:D:265:GLY:H	1.28	0.81
1:A:263:HIS:CD2	1:A:265:GLY:H	2.00	0.79
1:D:263:HIS:CD2	1:D:265:GLY:H	2.00	0.79
1:A:19:GLU:HG3	1:A:20:PRO:HD2	1.66	0.78
1:D:97:ARG:HH12	3:F:6:VAL:HG11	1.49	0.77
1:A:263:HIS:HD2	1:A:265:GLY:H	1.35	0.73
2:B:7:ILE:HD12	2:B:82:VAL:HG21	1.71	0.71
1:D:111:ARG:HD2	1:D:113:TYR:OH	1.93	0.69
1:D:97:ARG:HH22	3:F:6:VAL:HG13	1.58	0.67
1:A:97:ARG:NH2	4:A:2192:HOH:O	2.27	0.66
1:D:169:ARG:O	1:D:173:GLU:HG2	1.95	0.65
2:E:73:THR:HG22	2:E:76:ASP:HB2	1.79	0.65
1:D:97:ARG:HH12	3:F:6:VAL:CG1	2.10	0.64
1:A:58:GLU:OE1	4:A:2116:HOH:O	2.15	0.63
2:E:3:ARG:CZ	4:E:2013:HOH:O	2.47	0.62
1:A:197:HIS:O	4:A:2306:HOH:O	2.16	0.61

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:73:THR:CG2	2:E:76:ASP:H	2.13	0.61
2:B:7:ILE:CD1	2:B:27:VAL:HG12	2.31	0.61
1:A:251:SER:O	4:A:2365:HOH:O	2.16	0.60
1:D:97:ARG:NH2	3:F:6:VAL:HG13	2.15	0.60
3:C:9:LEU:OXT	4:C:2018:HOH:O	2.17	0.59
1:A:58:GLU:CG	4:A:2117:HOH:O	2.22	0.59
1:D:93:HIS:HD2	1:D:119:ASP:OD2	1.85	0.59
1:D:93:HIS:HE1	4:D:2178:HOH:O	1.85	0.58
1:D:97:ARG:HH21	1:D:114:HIS:HE1	1.50	0.58
1:A:93:HIS:HD2	1:A:119:ASP:OD2	1.87	0.57
2:E:73:THR:HG23	2:E:76:ASP:H	1.70	0.56
1:A:93:HIS:HE1	4:A:2176:HOH:O	1.87	0.56
1:D:201:LEU:HD12	1:D:249:VAL:HG21	1.87	0.56
2:E:83:ASN:HD21	2:E:90:PRO:HG3	1.72	0.55
1:D:19:GLU:OE1	1:D:75:ARG:NH2	2.40	0.55
1:D:131:ARG:HD3	4:D:2233:HOH:O	2.07	0.55
1:A:111:ARG:HD2	1:A:113:TYR:OH	2.07	0.54
1:A:19:GLU:HG2	4:A:2019:HOH:O	2.09	0.53
1:D:186:LYS:HD3	4:D:2298:HOH:O	2.10	0.51
1:D:74:HIS:CE1	4:D:2143:HOH:O	2.62	0.51
1:A:117:ALA:HB2	2:B:60:TRP:CE2	2.46	0.51
2:B:7:ILE:HD12	2:B:27:VAL:HG12	1.94	0.50
2:B:87:LEU:O	4:B:2153:HOH:O	2.20	0.49
1:D:82:ARG:NH1	4:D:2166:HOH:O	2.27	0.49
1:D:97:ARG:HH22	3:F:6:VAL:HG22	1.78	0.49
1:D:189:MET:HE2	1:D:274:TRP:HE3	1.78	0.49
1:D:260:HIS:CE1	4:D:2326:HOH:O	2.64	0.49
1:A:97:ARG:HE	1:A:114:HIS:HE1	1.62	0.48
2:B:85:VAL:HG13	4:B:2083:HOH:O	2.14	0.47
2:B:7:ILE:HD13	2:B:27:VAL:HG12	1.97	0.47
1:A:86:ASN:HB2	4:A:2169:HOH:O	2.14	0.47
1:D:216:THR:HG23	4:D:2354:HOH:O	2.14	0.46
2:E:75:LYS:HD3	4:E:2186:HOH:O	2.14	0.46
1:D:268:LYS:NZ	4:D:2400:HOH:O	2.48	0.46
1:A:6:ARG:HD3	4:A:2193:HOH:O	2.15	0.46
2:B:85:VAL:HG11	4:B:2003:HOH:O	2.16	0.45
2:B:4:THR:HG22	2:B:5:PRO:HD2	1.98	0.45
2:E:48:LYS:NZ	2:E:50:GLU:OE2	2.50	0.45
1:A:116:TYR:CZ	3:C:9:LEU:HD13	2.52	0.45
1:D:6:ARG:HD2	1:D:98:MET:SD	2.57	0.45
2:B:0:MET:HE3	2:B:0:MET:HB3	1.89	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:97:ARG:HE	1:D:114:HIS:CE1	2.34	0.44
3:F:3:TYR:OH	3:F:5:THR:HG23	2.18	0.44
2:B:0:MET:HG2	4:B:2001:HOH:O	2.18	0.43
1:D:117:ALA:HB2	2:E:60:TRP:CE2	2.54	0.43
1:D:253:GLN:NE2	1:D:256:ARG:HH11	2.16	0.43
2:E:3:ARG:NE	4:E:2013:HOH:O	2.51	0.43
1:D:97:ARG:NH1	3:F:6:VAL:CG1	2.80	0.43
1:D:97:ARG:NH1	3:F:6:VAL:HG11	2.26	0.42
2:B:97:ARG:HG3	2:B:98:ASP:OD1	2.19	0.42
2:B:98:ASP:HB3	4:B:2173:HOH:O	2.19	0.42
2:B:6:LYS:NZ	4:B:2024:HOH:O	2.51	0.42
1:A:97:ARG:HE	1:A:114:HIS:CE1	2.38	0.41
1:A:210:PRO:O	1:A:263:HIS:HE1	2.03	0.41
1:D:11:SER:HB2	1:D:74:HIS:HD2	1.85	0.41
1:A:253:GLN:NE2	1:A:256:ARG:HH11	2.18	0.41
1:A:201:LEU:HD12	1:A:249:VAL:HG11	2.01	0.41
2:E:69:GLU:HG3	4:E:2180:HOH:O	2.20	0.41
1:D:186:LYS:CD	4:D:2298:HOH:O	2.67	0.40
1:D:176:LYS:HE3	1:D:176:LYS:HB2	1.77	0.40
1:D:97:ARG:HH21	1:D:114:HIS:CE1	2.35	0.40
1:D:214:THR:HB	1:D:262:GLN:HB2	2.03	0.40

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	274/276 (99%)	268 (98%)	4 (2%)	2 (1%)	26	8
1	D	274/276 (99%)	271 (99%)	3 (1%)	0	100	100
2	B	98/100 (98%)	96 (98%)	2 (2%)	0	100	100
2	E	98/100 (98%)	97 (99%)	1 (1%)	0	100	100

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
3	F	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
All	All	758/770 (98%)	744 (98%)	12 (2%)	2 (0%)	46	23

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	275	GLU
1	A	194	VAL

### 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	226/232 (97%)	219 (97%)	7 (3%)	47	19
1	D	226/232 (97%)	223 (99%)	3 (1%)	76	56
2	B	91/95 (96%)	87 (96%)	4 (4%)	35	10
2	E	91/95 (96%)	89 (98%)	2 (2%)	60	31
3	C	8/8 (100%)	8 (100%)	0	100	100
3	F	8/8 (100%)	8 (100%)	0	100	100
All	All	650/670 (97%)	634 (98%)	16 (2%)	55	26

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	ARG
1	A	82	ARG
1	A	121	LYS
1	A	128	GLU
1	A	138	MET
1	A	156	LEU
1	A	163	THR
2	B	0	MET

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	B	70	PHE
2	B	75	LYS
2	B	98	ASP
1	D	19	GLU
1	D	74	HIS
1	D	88	SER
2	E	70	PHE
2	E	75	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	74	HIS
1	A	93	HIS
1	A	114	HIS
1	A	115	GLN
1	A	174	ASN
1	A	253	GLN
1	A	263	HIS
1	D	74	HIS
1	D	93	HIS
1	D	114	HIS
1	D	155	GLN
1	D	174	ASN
1	D	197	HIS
1	D	253	GLN
1	D	263	HIS
2	E	83	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 ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

There are no ligands in this entry.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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	276/276 (100%)	0.05	10 (3%) 46 43	12, 22, 32, 45	0
1	D	276/276 (100%)	0.02	11 (3%) 42 39	10, 21, 35, 42	0
2	B	100/100 (100%)	-0.10	4 (4%) 42 39	13, 21, 31, 35	0
2	E	100/100 (100%)	-0.25	2 (2%) 68 67	11, 16, 24, 30	0
3	C	9/9 (100%)	0.34	0 100 100	14, 23, 30, 33	0
3	F	9/9 (100%)	1.15	2 (22%) 1 1	16, 29, 32, 32	0
All	All	770/770 (100%)	-0.00	29 (3%) 44 41	10, 20, 32, 45	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	16	GLY	5.3
1	A	194	VAL	4.7
3	F	5	THR	4.3
1	A	196	ASP	4.0
1	A	275	GLU	3.7
1	D	86	ASN	3.4
2	B	48	LYS	3.2
1	A	195	SER	3.1
2	B	98	ASP	2.9
1	A	86	ASN	2.8
1	D	196	ASP	2.8
1	D	267	PRO	2.8
1	A	41	ALA	2.7
1	D	90	ALA	2.6
1	D	193	ALA	2.6
1	A	113	TYR	2.5
1	D	268	LYS	2.5
2	E	48	LYS	2.5
3	F	6	VAL	2.5

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	D	18	GLY	2.4
1	D	197	HIS	2.3
1	A	151	HIS	2.3
2	E	73	THR	2.2
1	A	255	GLN	2.2
1	D	194	VAL	2.2
2	B	89	GLN	2.1
1	D	195	SER	2.1
2	B	39	LEU	2.1
1	A	197	HIS	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 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.