



# Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 11:45 am BST

PDB ID : 5TEZ  
Title : TCR F50 recognizing M1-HLA-A2  
Authors : Yang, X.; Mariuzza, R.A.  
Deposited on : 2016-09-23  
Resolution : 1.70 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

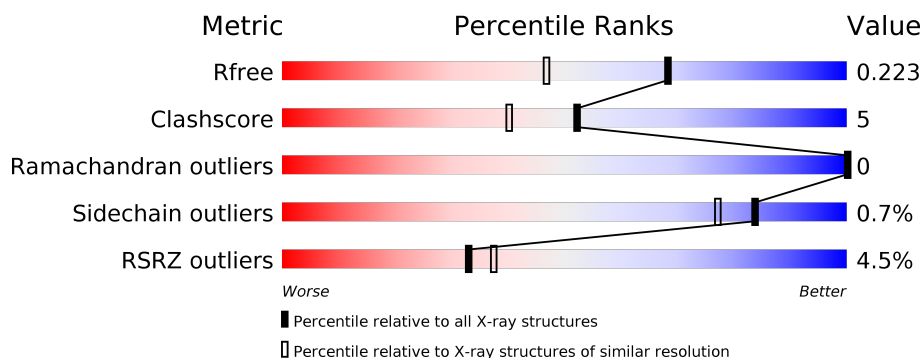
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.70 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	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

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	C	9	<div> <div>78%</div> <div>22%</div> </div>
2	A	275	<div>5%</div> <div>80%</div> <div>19%</div> <div>.</div>
3	B	100	<div>6%</div> <div>80%</div> <div>19%</div> <div>.</div>
4	I	208	<div>4%</div> <div>80%</div> <div>16%</div> <div>..</div>
5	J	243	<div>3%</div> <div>84%</div> <div>14%</div> <div>..</div>

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 7466 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 GLY-ILE-LEU-GLY-PHE-VAL-PHE-THR-LEU.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	C	9	Total	C	N	O	0	0	0
			68	49	9	10			

- Molecule 2 is a protein called HLA class I histocompatibility antigen, A-2 alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	275	Total	C	N	O	S	0	0	0
			2246	1403	409	425	9			

- Molecule 3 is a protein called Beta-2-microglobulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	B	100	Total	C	N	O	S	0	0	0
			834	531	141	159	3			

- Molecule 4 is a protein called TCR F50 alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	I	202	Total	C	N	O	S	0	0	0
			1586	992	268	319	7			

- Molecule 5 is a protein called TCR F50 beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	J	240	Total	C	N	O	S	0	0	0
			1927	1219	334	366	8			

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	C	4	Total	O	0	0
			4	4		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	246	Total 246	O 246	0	0
6	B	125	Total 125	O 125	0	0
6	I	187	Total 187	O 187	0	0
6	J	243	Total 243	O 243	0	0

### 3 Residue-property plots


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.

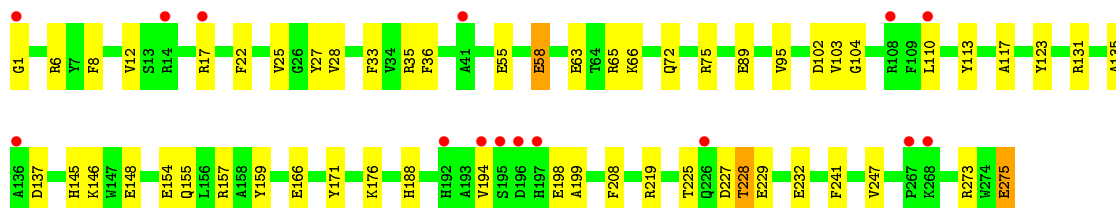
- Molecule 1: GLY-ILE-LEU-GLY-PHE-VAL-PHE-THR-LEU

Chain C: 




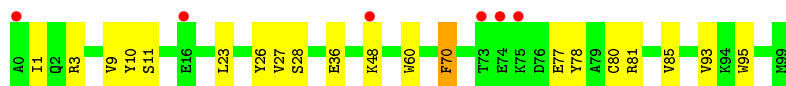
- Molecule 2: HLA class I histocompatibility antigen, A-2 alpha chain

Chain A: 




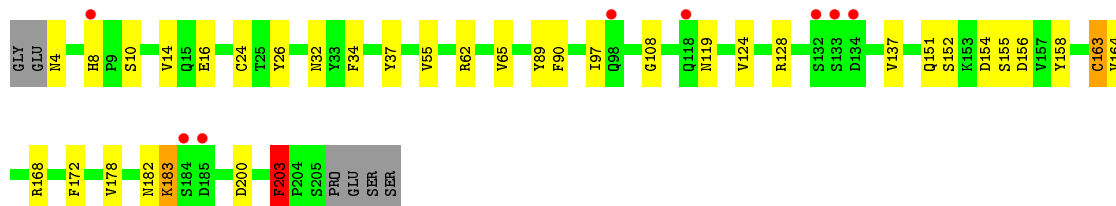
- Molecule 3: Beta-2-microglobulin

Chain B: 

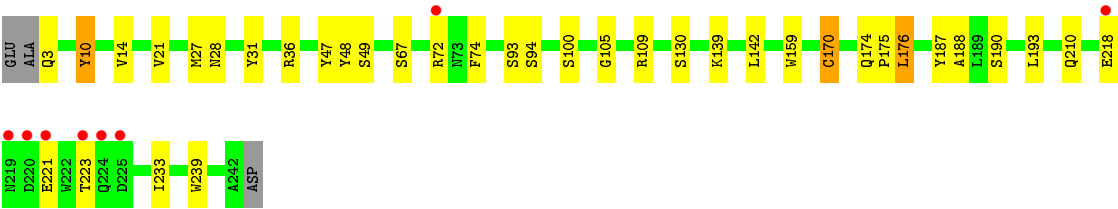
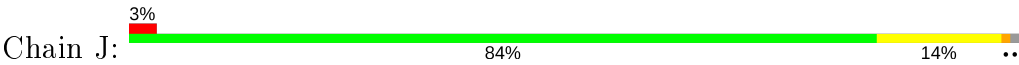


- Molecule 4: TCR F50 alpha chain

Chain I: 



- Molecule 5: TCR F50 beta chain



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	66.27Å 71.05Å 100.69Å 90.00° 96.22° 90.00°	Depositor
Resolution (Å)	37.92 – 1.70 37.92 – 1.70	Depositor EDS
% Data completeness (in resolution range)	98.1 (37.92-1.70) 98.1 (37.92-1.70)	Depositor EDS
$R_{merge}$	0.35	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.33 (at 1.70Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, $R_{free}$	0.190 , 0.224 0.192 , 0.223	Depositor DCC
$R_{free}$ test set	2000 reflections (1.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	20.3	Xtriage
Anisotropy	0.343	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 41.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	7466	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.75% 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	C	2.24	2/69 (2.9%)	0.89	0/90
2	A	2.06	37/2311 (1.6%)	0.90	1/3137 (0.0%)
3	B	2.06	15/857 (1.8%)	0.92	2/1159 (0.2%)
4	I	2.04	21/1619 (1.3%)	0.95	4/2195 (0.2%)
5	J	2.08	25/1980 (1.3%)	0.88	2/2696 (0.1%)
All	All	2.06	100/6836 (1.5%)	0.91	9/9277 (0.1%)

All (100) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	J	36	ARG	CB-CG	-10.82	1.23	1.52
4	I	14	VAL	CB-CG1	-9.31	1.33	1.52
2	A	135	ALA	CA-CB	-9.00	1.33	1.52
2	A	275	GLU	CG-CD	-8.55	1.39	1.51
2	A	27	TYR	CD2-CE2	-8.48	1.26	1.39
4	I	155	SER	CB-OG	-8.00	1.31	1.42
3	B	9	VAL	CB-CG2	-7.42	1.37	1.52
4	I	163	CYS	CB-SG	-7.17	1.70	1.82
2	A	275	GLU	CB-CG	-7.11	1.38	1.52
5	J	239	TRP	CE3-CZ3	-6.87	1.26	1.38
2	A	25	VAL	CB-CG2	-6.80	1.38	1.52
2	A	247	VAL	CB-CG1	-6.71	1.38	1.52
4	I	164	VAL	CB-CG2	-6.68	1.38	1.52
5	J	21	VAL	CB-CG2	-6.60	1.39	1.52
5	J	67	SER	CB-OG	-6.54	1.33	1.42
5	J	48	TYR	CD2-CE2	-6.54	1.29	1.39
2	A	113	TYR	CD1-CE1	-6.38	1.29	1.39
2	A	275	GLU	CD-OE2	-6.34	1.18	1.25
4	I	65	VAL	CB-CG2	-6.33	1.39	1.52
5	J	130	SER	CB-OG	-6.29	1.34	1.42
4	I	183	LYS	CG-CD	-6.26	1.31	1.52
4	I	137	VAL	CB-CG2	-6.24	1.39	1.52
3	B	77	GLU	CG-CD	-6.23	1.42	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	78	TYR	CD1-CE1	-6.20	1.30	1.39
2	A	166	GLU	CD-OE2	-6.16	1.18	1.25
3	B	70	PHE	CD1-CE1	-6.14	1.26	1.39
4	I	16	GLU	CB-CG	-6.06	1.40	1.52
2	A	146	LYS	CB-CG	-6.05	1.36	1.52
2	A	228	THR	CB-CG2	-6.04	1.32	1.52
2	A	123	TYR	CD2-CE2	-5.96	1.30	1.39
4	I	26	TYR	CD2-CE2	-5.93	1.30	1.39
5	J	100	SER	CB-OG	-5.91	1.34	1.42
3	B	93	VAL	CB-CG1	-5.90	1.40	1.52
4	I	55	VAL	CB-CG1	-5.87	1.40	1.52
5	J	170	CYS	CB-SG	-5.84	1.72	1.81
2	A	103	VAL	CB-CG2	-5.83	1.40	1.52
2	A	176	LYS	CB-CG	-5.82	1.36	1.52
2	A	208	PHE	CD2-CE2	-5.80	1.27	1.39
2	A	148	GLU	CD-OE1	-5.78	1.19	1.25
2	A	199	ALA	CA-CB	-5.74	1.40	1.52
2	A	229	GLU	CD-OE1	-5.73	1.19	1.25
5	J	187	TYR	CE1-CZ	-5.72	1.31	1.38
5	J	47	TYR	CD2-CE2	-5.69	1.30	1.39
5	J	93	SER	CB-OG	-5.68	1.34	1.42
3	B	10	TYR	CE1-CZ	-5.67	1.31	1.38
2	A	22	PHE	CD2-CE2	-5.62	1.28	1.39
3	B	85	VAL	CB-CG1	-5.61	1.41	1.52
3	B	80	CYS	CB-SG	-5.60	1.72	1.81
5	J	105	GLY	C-O	-5.59	1.14	1.23
4	I	34	PHE	CE2-CZ	-5.57	1.26	1.37
5	J	74	PHE	CE2-CZ	-5.56	1.26	1.37
4	I	203	PHE	CG-CD2	-5.53	1.30	1.38
2	A	159	TYR	CE2-CZ	-5.53	1.31	1.38
3	B	95	TRP	CE3-CZ3	-5.52	1.29	1.38
2	A	33	PHE	CE1-CZ	-5.51	1.26	1.37
4	I	16	GLU	CD-OE2	-5.50	1.19	1.25
2	A	154	GLU	CB-CG	-5.48	1.41	1.52
4	I	37	TYR	CD1-CE1	-5.47	1.31	1.39
3	B	81	ARG	CD-NE	-5.47	1.37	1.46
3	B	26	TYR	CD1-CE1	-5.46	1.31	1.39
5	J	14	VAL	CB-CG1	-5.45	1.41	1.52
2	A	12	VAL	CB-CG2	-5.44	1.41	1.52
2	A	159	TYR	CD2-CE2	-5.44	1.31	1.39
5	J	159	TRP	CE3-CZ3	-5.43	1.29	1.38
2	A	171	TYR	CG-CD1	-5.39	1.32	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	232	GLU	CD-OE2	-5.39	1.19	1.25
5	J	190	SER	CB-OG	-5.37	1.35	1.42
4	I	55	VAL	C-O	-5.36	1.13	1.23
2	A	8	PHE	C-O	-5.33	1.13	1.23
5	J	31	TYR	CD1-CE1	-5.33	1.31	1.39
2	A	27	TYR	CD1-CE1	-5.30	1.31	1.39
5	J	49	SER	CB-OG	-5.29	1.35	1.42
5	J	223	THR	CB-CG2	-5.29	1.34	1.52
4	I	89	TYR	CD2-CE2	-5.28	1.31	1.39
5	J	10	TYR	CD2-CE2	-5.26	1.31	1.39
4	I	16	GLU	CD-OE1	-5.25	1.19	1.25
3	B	28	SER	CB-OG	-5.24	1.35	1.42
4	I	90	PHE	CE1-CZ	-5.19	1.27	1.37
2	A	123	TYR	CD1-CE1	-5.19	1.31	1.39
4	I	24	CYS	CB-SG	-5.18	1.73	1.81
1	C	7	PHE	CE2-CZ	-5.17	1.27	1.37
5	J	48	TYR	CD1-CE1	-5.14	1.31	1.39
5	J	188	ALA	CA-CB	-5.14	1.41	1.52
4	I	178	VAL	CB-CG1	-5.13	1.42	1.52
1	C	5	PHE	CE1-CZ	-5.12	1.27	1.37
4	I	108	GLY	C-O	-5.12	1.15	1.23
2	A	241	PHE	CD1-CE1	-5.10	1.29	1.39
2	A	28	VAL	C-O	-5.10	1.13	1.23
2	A	36	PHE	CE2-CZ	-5.10	1.27	1.37
5	J	94	SER	C-O	-5.09	1.13	1.23
3	B	11	SER	CB-OG	-5.08	1.35	1.42
2	A	208	PHE	CE1-CZ	-5.08	1.27	1.37
2	A	65	ARG	C-O	-5.08	1.13	1.23
2	A	95	VAL	CB-CG2	-5.07	1.42	1.52
5	J	31	TYR	CD2-CE2	-5.05	1.31	1.39
3	B	81	ARG	CZ-NH2	-5.04	1.26	1.33
3	B	27	VAL	CB-CG1	-5.03	1.42	1.52
2	A	55	GLU	CD-OE1	-5.03	1.20	1.25
2	A	58	GLU	CB-CG	-5.01	1.42	1.52
5	J	193	LEU	C-O	-5.00	1.13	1.23

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	I	62	ARG	NE-CZ-NH2	-11.08	114.76	120.30
4	I	62	ARG	NE-CZ-NH1	10.65	125.62	120.30
3	B	81	ARG	NE-CZ-NH2	-9.21	115.70	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	81	ARG	NE-CZ-NH1	8.91	124.76	120.30
5	J	176	LEU	CA-CB-CG	7.61	132.81	115.30
5	J	36	ARG	NE-CZ-NH2	-6.41	117.09	120.30
4	I	183	LYS	CD-CE-NZ	-6.08	97.71	111.70
4	I	168	ARG	NE-CZ-NH1	5.44	123.02	120.30
2	A	110	LEU	CA-CB-CG	5.42	127.76	115.30

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	C	68	0	75	0	0
2	A	2246	0	2096	31	0
3	B	834	0	799	6	0
4	I	1586	0	1523	27	0
5	J	1927	0	1849	18	0
6	A	246	0	0	12	2
6	B	125	0	0	3	1
6	C	4	0	0	0	0
6	I	187	0	0	7	3
6	J	243	0	0	3	0
All	All	7466	0	6342	70	3

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 (70) 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:A:58:GLU:HG2	6:A:359:HOH:O	1.44	1.18
2:A:35:ARG:NH1	6:A:301:HOH:O	2.00	0.95
2:A:75:ARG:NH1	6:A:302:HOH:O	2.08	0.86
4:I:156:ASP:OD2	4:I:183:LYS:NZ	2.11	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:154:ASP:OD2	6:I:301:HOH:O	1.97	0.83
2:A:1:GLY:N	6:A:303:HOH:O	2.10	0.82
4:I:163:CYS:HG	5:J:170:CYS:CB	1.97	0.78
5:J:109:ARG:NH2	6:J:301:HOH:O	2.15	0.77
3:B:3:ARG:NH2	6:B:101:HOH:O	2.04	0.76
4:I:182:ASN:ND2	6:I:306:HOH:O	2.21	0.73
4:I:119:ASN:OD1	6:I:302:HOH:O	2.06	0.72
2:A:58:GLU:CD	2:A:58:GLU:H	1.94	0.69
4:I:124:VAL:HB	4:I:203:PHE:CD2	2.27	0.68
2:A:17:ARG:NH1	2:A:89:GLU:OE2	2.26	0.68
4:I:154:ASP:OD1	6:I:304:HOH:O	2.12	0.67
4:I:124:VAL:HB	4:I:203:PHE:CE2	2.30	0.66
4:I:163:CYS:CB	5:J:170:CYS:HG	2.07	0.66
2:A:72:GLN:OE1	2:A:75:ARG:NH2	2.32	0.63
2:A:17:ARG:NH1	2:A:89:GLU:CD	2.53	0.62
2:A:137:ASP:HB3	6:A:307:HOH:O	2.00	0.62
4:I:158:TYR:CD1	5:J:176:LEU:HD21	2.35	0.61
4:I:4:ASN:HA	6:I:314:HOH:O	2.00	0.60
2:A:58:GLU:OE1	6:A:304:HOH:O	2.16	0.60
2:A:273:ARG:NE	2:A:275:GLU:OE2	2.29	0.60
2:A:17:ARG:NE	2:A:89:GLU:OE1	2.36	0.59
5:J:10:TYR:CE1	5:J:109:ARG:HD2	2.39	0.57
2:A:275:GLU:HG2	6:A:326:HOH:O	2.03	0.57
4:I:151:GLN:HG2	4:I:152:SER:N	2.22	0.54
4:I:151:GLN:HG2	4:I:152:SER:H	1.72	0.54
2:A:145:HIS:HE1	6:A:441:HOH:O	1.91	0.53
4:I:8:HIS:O	6:I:305:HOH:O	2.19	0.53
3:B:3:ARG:NH1	6:B:103:HOH:O	2.29	0.53
2:A:188:HIS:HD2	6:A:394:HOH:O	1.92	0.53
4:I:163:CYS:CB	5:J:170:CYS:SG	2.95	0.51
4:I:163:CYS:HB3	5:J:170:CYS:SG	2.51	0.51
5:J:72:ARG:NH1	6:J:308:HOH:O	2.44	0.49
4:I:128:ARG:HD2	6:I:319:HOH:O	2.11	0.49
4:I:124:VAL:CB	4:I:203:PHE:CE2	2.95	0.49
2:A:17:ARG:CZ	2:A:89:GLU:CD	2.81	0.48
5:J:221:GLU:CD	5:J:221:GLU:H	2.16	0.48
2:A:219:ARG:CZ	2:A:219:ARG:HB3	2.43	0.48
4:I:156:ASP:OD2	4:I:183:LYS:CE	2.61	0.48
3:B:48:LYS:HG3	3:B:48:LYS:O	2.15	0.47
2:A:225:THR:O	2:A:228:THR:HB	2.15	0.47
2:A:227:ASP:OD1	2:A:227:ASP:N	2.47	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:104:GLY:HA3	6:A:400:HOH:O	2.16	0.46
5:J:3:GLN:N	6:J:314:HOH:O	2.49	0.46
2:A:194:VAL:HG22	2:A:198:GLU:HB2	1.98	0.45
2:A:131:ARG:HH21	2:A:157:ARG:NH2	2.15	0.45
2:A:117:ALA:HB2	3:B:60:TRP:CE2	2.52	0.44
4:I:163:CYS:HB3	5:J:170:CYS:HG	1.79	0.44
2:A:75:ARG:NH2	6:A:317:HOH:O	2.50	0.44
2:A:63:GLU:OE2	2:A:66:LYS:NZ	2.47	0.44
3:B:23:LEU:HB2	3:B:70:PHE:CD1	2.54	0.43
5:J:210:GLN:HG3	5:J:233:ILE:HG23	1.99	0.43
2:A:17:ARG:NH1	2:A:89:GLU:OE1	2.51	0.43
2:A:75:ARG:HH11	2:A:75:ARG:HG2	1.84	0.42
2:A:17:ARG:HH11	2:A:89:GLU:CD	2.23	0.42
4:I:163:CYS:SG	5:J:170:CYS:CB	3.02	0.42
2:A:155:GLN:OE1	4:I:32:ASN:HB2	2.20	0.42
3:B:36:GLU:OE2	6:B:102:HOH:O	2.22	0.41
4:I:200:ASP:OD1	4:I:200:ASP:N	2.45	0.41
4:I:97:ILE:HD13	4:I:97:ILE:HG21	1.61	0.41
4:I:163:CYS:HG	5:J:170:CYS:HG	0.83	0.41
5:J:27:MET:O	5:J:28:ASN:HB3	2.21	0.41
4:I:172:PHE:CE2	5:J:139:LYS:HE2	2.56	0.41
2:A:137:ASP:HB2	6:A:413:HOH:O	2.19	0.41
4:I:163:CYS:SG	5:J:170:CYS:HB2	2.61	0.41
5:J:174:GLN:HA	5:J:175:PRO:HD3	1.87	0.40
2:A:6:ARG:NH2	2:A:102:ASP:OD1	2.52	0.40

All (3) 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)
6:A:528:HOH:O	6:I:377:HOH:O[1_455]	2.07	0.13
6:B:194:HOH:O	6:I:453:HOH:O[1_455]	2.12	0.08
6:A:454:HOH:O	6:I:471:HOH:O[2_8411]	2.19	0.01

## 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	C	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
2	A	273/275 (99%)	267 (98%)	6 (2%)	0	100	100
3	B	98/100 (98%)	96 (98%)	2 (2%)	0	100	100
4	I	200/208 (96%)	195 (98%)	5 (2%)	0	100	100
5	J	238/243 (98%)	234 (98%)	4 (2%)	0	100	100
All	All	816/835 (98%)	798 (98%)	18 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	C	7/7 (100%)	7 (100%)	0	100	100
2	A	231/231 (100%)	231 (100%)	0	100	100
3	B	94/94 (100%)	93 (99%)	1 (1%)	73	63
4	I	182/187 (97%)	180 (99%)	2 (1%)	73	63
5	J	213/215 (99%)	211 (99%)	2 (1%)	78	70
All	All	727/734 (99%)	722 (99%)	5 (1%)	84	77

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	B	1	ILE
4	I	10	SER
4	I	203	PHE
5	J	142	LEU
5	J	218	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	145	HIS
2	A	188	HIS
3	B	13	HIS
4	I	119	ASN
4	I	182	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 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	C	9/9 (100%)	0.53	0 <span>100</span> <span>100</span>	15, 17, 20, 22	0
2	A	275/275 (100%)	0.32	15 (5%) <span>25</span> <span>27</span>	14, 23, 40, 50	0
3	B	100/100 (100%)	0.37	6 (6%) <span>21</span> <span>24</span>	15, 22, 42, 47	0
4	I	202/208 (97%)	0.24	8 (3%) <span>38</span> <span>42</span>	14, 21, 39, 59	0
5	J	240/243 (98%)	0.07	8 (3%) <span>46</span> <span>51</span>	15, 21, 35, 57	0
All	All	826/835 (98%)	0.24	37 (4%) <span>33</span> <span>37</span>	14, 22, 39, 59	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	I	133	SER	7.9
2	A	194	VAL	6.1
5	J	223	THR	5.5
4	I	134	ASP	4.6
5	J	218	GLU	4.4
5	J	225	ASP	4.0
5	J	219	ASN	3.9
2	A	41	ALA	3.8
2	A	267	PRO	3.8
4	I	132	SER	3.5
4	I	8	HIS	3.5
2	A	197	HIS	3.4
2	A	196	ASP	3.3
2	A	195	SER	3.1
2	A	17	ARG	3.1
4	I	185	ASP	2.9
5	J	221	GLU	2.8
2	A	268	LYS	2.7
2	A	1	GLY	2.6
3	B	16	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
5	J	224	GLN	2.5
3	B	48	LYS	2.5
2	A	14	ARG	2.5
2	A	226	GLN	2.5
3	B	73	THR	2.4
2	A	108	ARG	2.4
5	J	220	ASP	2.3
4	I	98	GLN	2.3
3	B	74	GLU	2.2
2	A	136	ALA	2.2
4	I	184	SER	2.2
3	B	75	LYS	2.2
3	B	0	ALA	2.1
5	J	72	ARG	2.1
2	A	192	HIS	2.1
4	I	118	GLN	2.1
2	A	110	LEU	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.