



# Full wwPDB X-ray Structure Validation Report i

Mar 20, 2024 – 12:05 PM EDT

PDB ID : 8EN8  
Title : Cross-reactive 3180 TCR recognition of HLA-B\*35:01-NP4 epitope from 1972 influenza strain  
Authors : Littler, D.R.; Rossjohn, J.  
Deposited on : 2022-09-29  
Resolution : 2.70 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 i 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 ①) were used in the production of this report:

MolProbity : 4.02b-467  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
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) : 2.36

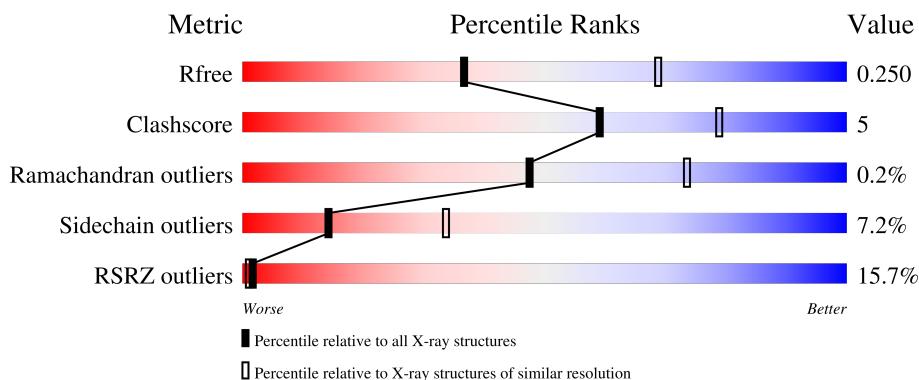
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## X-RAY DIFFRACTION

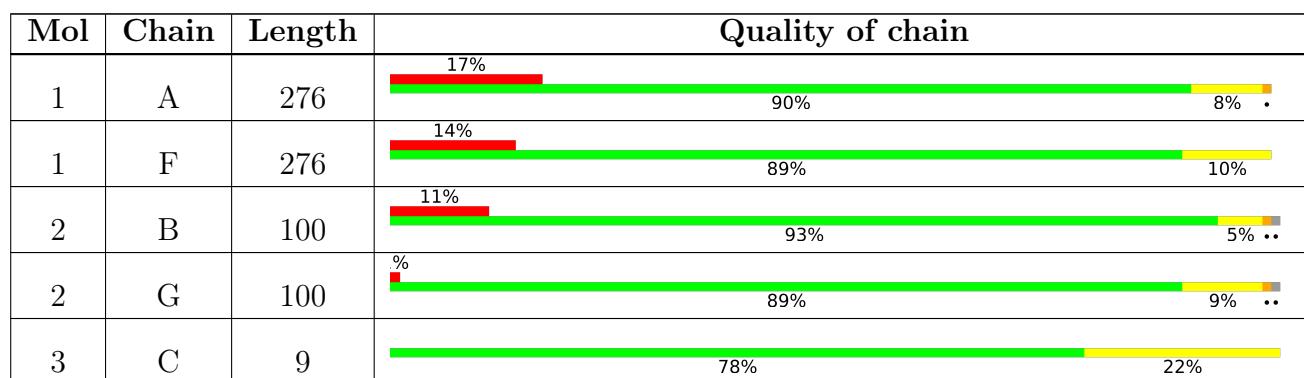
The reported resolution of this entry is 2.70 Å.

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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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 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.



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Mol	Chain	Length	Quality of chain	
3	H	9	67%	33%
4	D	205	4% 89%	11%
4	I	205	31% 87%	11% •
5	E	245	5% 82%	16% •
5	J	245	32% 76%	21% •

## 2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 13859 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 MHC class I antigen.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	276	Total	C	N	O	S	0	1	0
			2262	1409	413	433	7			

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	F	276	Total	C	N	O	S	0	1	0
			2262	1409	413	433	7			

- 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
			829	528	140	158	3			

2	G	99	Total	C	N	O	S	0	0	0
			829	528	140	158	3			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	MET	-	initiating methionine	UNP P61769
G	0	MET	-	initiating methionine	UNP P61769

- Molecule 3 is a protein called Nucleoprotein NP4 epitope.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	9	Total	C	N	O	S	0	0	0
			73	48	10	14	1			

3	H	9	Total	C	N	O	S	0	0	0
			73	48	10	14	1			

- Molecule 4 is a protein called 3180 TCR alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	205	Total	C	N	O	S	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	I	205	Total	C 1594	N 994	O 266	S 326	8	0	0

- Molecule 5 is a protein called 3180 TCR beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	245	Total	C 1937	N 1219	O 334	S 375	9	0	0
5	J	245	Total	C 1937	N 1219	O 334	S 375	9	0	0

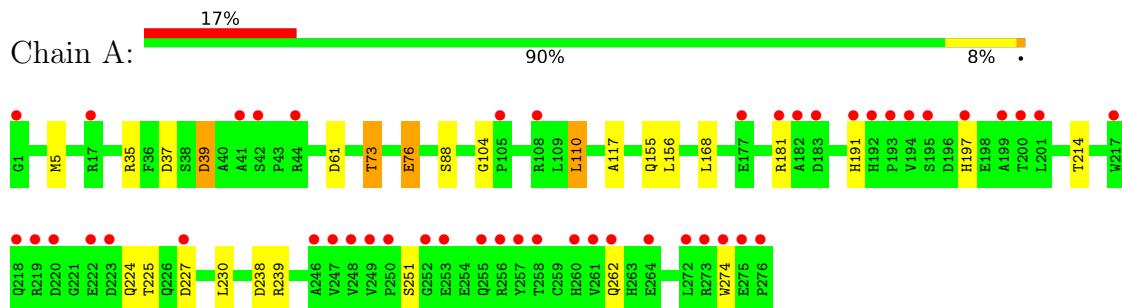
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	79	Total	O 79	0	0
6	B	14	Total	O 14	0	0
6	C	3	Total	O 3	0	0
6	D	51	Total	O 51	0	0
6	E	80	Total	O 80	0	0
6	F	110	Total	O 110	0	0
6	G	36	Total	O 36	0	0
6	H	8	Total	O 8	0	0
6	I	34	Total	O 34	0	0
6	J	54	Total	O 54	0	0

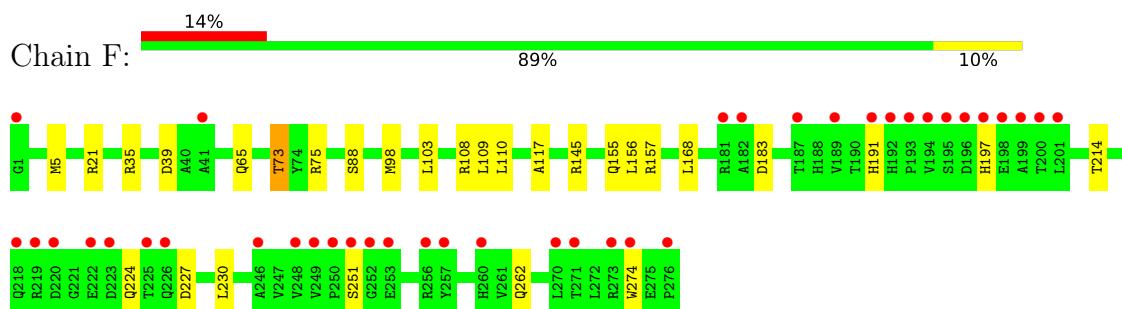
### 3 Residue-property plots

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.

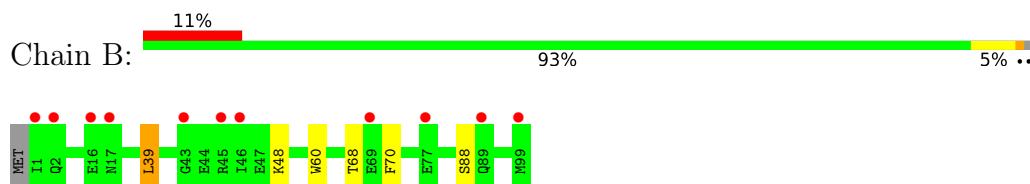
- Molecule 1: MHC class I antigen



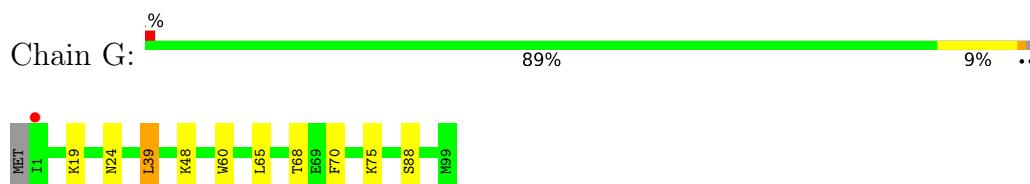
- Molecule 1: MHC class I antigen



- Molecule 2: Beta-2-microglobulin

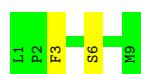


- Molecule 2: Beta-2-microglobulin



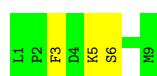
- Molecule 3: Nucleoprotein NP4 epitope

Chain C:  78%  22%



- Molecule 3: Nucleoprotein NP4 epitope

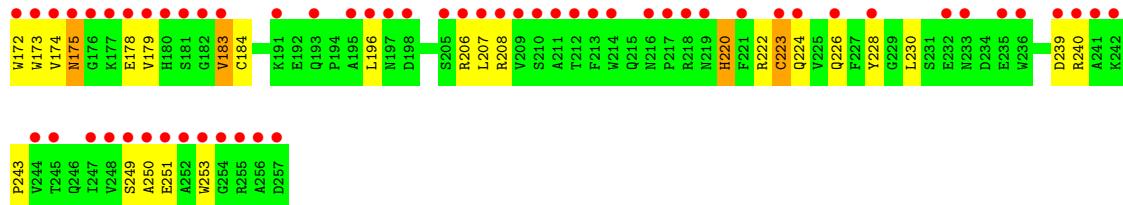
Chain H:  67%  33%



- Molecule 4: 3180 TCR alpha chain

Chain D:  89%  4%  11%





## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	79.77Å 116.69Å 253.18Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	27.20 – 2.70 27.20 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.9 (27.20-2.70) 100.0 (27.20-2.70)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) >$ <sup>1</sup>	2.12 (at 2.72Å)	Xtriage
Refinement program	BUSTER, PHENIX 1.10.1_2155	Depositor
$R$ , $R_{free}$	0.207 , 0.249 0.211 , 0.250	Depositor DCC
$R_{free}$ test set	3281 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	46.2	Xtriage
Anisotropy	0.458	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 61.9	EDS
L-test for twinning <sup>2</sup>	$<  L  > = 0.48$ , $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	13859	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	83.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.90% 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  $< |L| >$ ,  $< L^2 >$  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	0.45	0/2325	0.65	0/3161
1	F	0.47	0/2325	0.64	0/3161
2	B	0.43	0/852	0.62	0/1152
2	G	0.42	0/852	0.64	0/1152
3	C	0.67	0/74	0.68	0/97
3	H	0.40	0/74	0.67	0/97
4	D	0.41	0/1628	0.64	0/2205
4	I	0.42	0/1628	0.63	0/2205
5	E	0.40	0/1988	0.68	0/2705
5	J	0.45	0/1988	0.70	0/2705
All	All	0.44	0/13734	0.66	0/18640

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	2262	0	2122	13	0
1	F	2262	0	2122	10	0
2	B	829	0	794	2	0
2	G	829	0	794	3	0
3	C	73	0	78	2	0
3	H	73	0	78	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	1594	0	1521	7	0
4	I	1594	0	1521	23	0
5	E	1937	0	1856	30	0
5	J	1937	0	1856	57	0
6	A	79	0	0	0	0
6	B	14	0	0	0	0
6	C	3	0	0	0	0
6	D	51	0	0	0	0
6	E	80	0	0	2	0
6	F	110	0	0	1	0
6	G	36	0	0	0	0
6	H	8	0	0	0	0
6	I	34	0	0	1	0
6	J	54	0	0	0	0
All	All	13859	0	12742	124	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 (124) 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)
5:J:147:GLU:O	5:J:148:ILE:CG1	1.95	1.14
5:J:147:GLU:O	5:J:148:ILE:HG12	1.52	1.08
4:I:127:PRO:HG3	4:I:176:VAL:HG11	1.40	1.03
5:J:175:ASN:H	5:J:220:HIS:HD2	1.08	1.00
5:J:147:GLU:C	5:J:148:ILE:HG12	1.77	1.00
5:J:147:GLU:O	5:J:148:ILE:HG13	1.67	0.93
5:J:175:ASN:N	5:J:220:HIS:HD2	1.69	0.89
5:J:140:VAL:HG23	5:J:158:CYS:SG	2.15	0.86
4:I:176:VAL:HG12	4:I:187:ASN:OD1	1.82	0.80
5:J:175:ASN:N	5:J:220:HIS:CD2	2.52	0.77
5:J:175:ASN:H	5:J:220:HIS:CD2	2.00	0.74
5:E:46:PRO:O	5:E:48:GLN:NE2	2.22	0.73
4:I:214:PHE:HE2	5:J:146:ALA:HB1	1.53	0.72
5:J:142:GLU:HB2	5:J:143:PRO:HD2	1.71	0.71
5:J:173:TRP:CZ2	5:J:178:GLU:HG3	2.25	0.70
5:E:72:GLU:HB3	6:E:301:HOH:O	1.92	0.69
5:J:175:ASN:CA	5:J:220:HIS:CD2	2.76	0.68
5:E:157:VAL:HG12	5:E:206:ARG:HG2	1.78	0.66
5:J:175:ASN:HA	5:J:220:HIS:CD2	2.30	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:48:GLN:HE21	5:E:48:GLN:N	1.96	0.64
5:J:72:GLU:H	5:J:72:GLU:CD	2.02	0.64
5:J:183:VAL:HG13	5:J:207:LEU:HB2	1.79	0.63
5:E:39:MET:HG3	5:E:80:HIS:HE1	1.65	0.62
3:H:5:LYS:HE3	5:J:114:ASP:OD1	2.00	0.62
4:I:137:TYR:CE1	5:J:146:ALA:HB3	2.34	0.62
5:J:157:VAL:HG12	5:J:206:ARG:HG2	1.82	0.62
1:F:98:MET:HE2	6:F:375:HOH:O	1.99	0.61
5:J:158:CYS:HB2	5:J:172:TRP:CZ2	2.35	0.61
4:I:141:ASP:HB3	4:I:145:SER:H	1.65	0.61
4:I:137:TYR:HB3	5:J:144:SER:CB	2.32	0.60
5:E:24:ARG:HH11	5:E:85:THR:CG2	2.15	0.59
5:J:24:ARG:HH11	5:J:85:THR:CG2	2.15	0.59
5:J:151:THR:O	5:J:152:GLN:HB2	2.02	0.58
5:E:58:GLU:HG2	5:E:80:HIS:HD2	1.67	0.58
1:F:73:THR:HG21	3:H:6:SER:OG	2.04	0.57
1:A:181:ARG:HH21	1:A:239:ARG:HH21	1.51	0.57
5:J:148:ILE:HG23	5:J:154:ALA:HB2	1.86	0.56
5:J:174:VAL:HG23	5:J:179:VAL:HG21	1.87	0.56
5:E:39:MET:HG3	5:E:80:HIS:CE1	2.41	0.56
4:I:139:LEU:HD12	5:J:144:SER:HB2	1.88	0.56
5:J:167:HIS:HB3	5:J:228:TYR:HB2	1.89	0.55
5:J:224:GLN:NE2	5:J:226:GLN:HB2	2.21	0.55
4:I:139:LEU:HD22	5:J:157:VAL:HG22	1.89	0.55
5:E:58:GLU:HG2	5:E:80:HIS:CD2	2.41	0.55
5:J:223:CYS:HB3	5:J:250:ALA:O	2.07	0.54
1:F:155:GLN:HB3	3:H:3:PHE:HZ	1.72	0.54
1:A:155:GLN:HB3	3:C:3:PHE:HZ	1.73	0.54
4:I:214:PHE:CE2	5:J:146:ALA:HB1	2.39	0.53
5:E:58:GLU:HG3	5:E:84:LEU:HD13	1.90	0.53
1:A:37:ASP:OD1	1:A:39:ASP:HB2	2.09	0.53
4:I:137:TYR:CE1	5:J:146:ALA:O	2.62	0.53
5:J:183:VAL:CG1	5:J:207:LEU:HB2	2.38	0.53
5:E:230:LEU:HD12	5:E:243:PRO:HD2	1.90	0.52
1:A:73:THR:HG21	3:C:6:SER:OG	2.10	0.52
5:J:230:LEU:HD12	5:J:243:PRO:HD2	1.92	0.52
1:F:108:ARG:HG2	1:F:109:LEU:H	1.76	0.51
5:E:48:GLN:HE21	5:E:48:GLN:CA	2.23	0.50
5:J:148:ILE:CG2	5:J:154:ALA:HB2	2.41	0.50
1:A:104:GLY:HA2	1:A:110:LEU:HD12	1.93	0.49
1:A:5:MET:HB2	1:A:168:LEU:HD13	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:5:MET:HB2	1:F:168:LEU:HD13	1.94	0.49
5:J:147:GLU:C	5:J:149:SER:H	2.15	0.49
5:E:45:PHE:HB3	5:E:46:PRO:HD2	1.94	0.48
4:D:205:ASN:O	4:D:209:ILE:HG12	2.13	0.48
4:D:177:LEU:HB3	5:E:184:CYS:HB3	1.94	0.47
1:A:76:GLU:HA	1:A:76:GLU:OE1	2.13	0.47
1:A:181:ARG:NH2	1:A:239:ARG:HH21	2.12	0.47
5:J:175:ASN:CA	5:J:220:HIS:HD2	2.22	0.47
5:E:145:GLU:H	5:E:145:GLU:CD	2.17	0.47
1:A:117:ALA:HB2	2:B:60:TRP:CE2	2.50	0.46
4:I:37:ASN:HB2	6:I:308:HOH:O	2.15	0.46
4:I:216:PRO:HG3	5:J:146:ALA:HB3	1.97	0.46
4:I:137:TYR:CZ	5:J:146:ALA:O	2.69	0.46
5:E:48:GLN:NE2	5:E:48:GLN:CA	2.79	0.46
1:F:224:GLN:HB3	1:F:227:ASP:HB2	1.98	0.46
5:E:10:ARG:HG2	5:E:123:ARG:HB3	1.98	0.46
4:I:137:TYR:HB3	5:J:144:SER:OG	2.15	0.46
4:I:139:LEU:CD1	5:J:144:SER:HB2	2.45	0.46
5:J:39:MET:HG3	5:J:80:HIS:CE1	2.51	0.45
1:F:21:ARG:HG3	1:F:39:ASP:HB2	1.98	0.45
4:I:137:TYR:HB3	5:J:144:SER:HB3	1.99	0.45
1:A:238:ASP:O	1:A:239:ARG:HG2	2.16	0.45
4:D:190:VAL:HG23	5:E:206:ARG:HH11	1.81	0.45
5:E:43:ARG:HD2	6:E:309:HOH:O	2.17	0.45
1:A:224:GLN:HB3	1:A:227:ASP:HB2	1.99	0.45
4:D:169:VAL:HG12	4:D:193:SER:HB2	1.99	0.45
5:J:173:TRP:CE2	5:J:178:GLU:HG3	2.52	0.45
4:D:149:VAL:HG21	5:E:157:VAL:HG21	1.99	0.44
2:G:24:ASN:HB3	2:G:65:LEU:HD11	1.99	0.44
4:I:216:PRO:HG3	5:J:146:ALA:CB	2.48	0.44
5:J:45:PHE:HB3	5:J:46:PRO:HD2	2.00	0.44
1:A:214:THR:HB	1:A:262:GLN:HB3	1.99	0.44
4:I:134:PRO:O	4:I:213:THR:HA	2.18	0.44
5:J:222:ARG:HG3	5:J:251:GLU:HB3	1.99	0.44
1:F:117:ALA:HB2	2:G:60:TRP:CE2	2.53	0.43
5:E:24:ARG:HH11	5:E:85:THR:HG23	1.84	0.43
4:D:101:VAL:HG22	4:D:122:LYS:HD2	2.00	0.43
4:I:137:TYR:CD1	5:J:146:ALA:HB3	2.53	0.43
5:J:174:VAL:HG12	5:J:175:ASN:ND2	2.34	0.43
4:I:134:PRO:HG3	4:I:210:PRO:HG2	2.00	0.43
2:B:39:LEU:HD23	2:B:68:THR:HG22	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:184:PHE:HE2	5:J:208:ARG:NH1	2.16	0.43
1:A:191:HIS:HB2	1:A:274:TRP:NE1	2.34	0.42
4:I:153:THR:HG21	5:J:147:GLU:OE1	2.18	0.42
5:E:24:ARG:HD3	5:E:85:THR:HG23	2.00	0.42
5:E:141:PHE:HB2	5:E:157:VAL:CG2	2.50	0.42
5:J:183:VAL:HG13	5:J:207:LEU:HD13	2.00	0.42
5:J:142:GLU:CB	5:J:143:PRO:HD2	2.45	0.42
1:F:214:THR:HB	1:F:262:GLN:HB3	2.01	0.42
5:J:24:ARG:CD	5:J:85:THR:HG23	2.50	0.42
5:J:24:ARG:HD3	5:J:85:THR:HG23	2.02	0.41
5:E:146:ALA:O	5:E:150:HIS:HB2	2.20	0.41
5:E:19:VAL:HG11	5:E:124:LEU:HD11	2.02	0.41
5:E:24:ARG:CD	5:E:85:THR:HG23	2.50	0.41
5:J:223:CYS:O	5:J:223:CYS:SG	2.79	0.41
5:J:140:VAL:HG21	5:J:223:CYS:HB3	2.02	0.41
5:E:48:GLN:NE2	5:E:48:GLN:HA	2.36	0.41
5:E:54:ALA:HB3	5:E:78:ILE:CD1	2.50	0.41
2:G:39:LEU:HD23	2:G:68:THR:HG22	2.02	0.41
5:E:169:GLU:HG3	5:E:226:GLN:HB3	2.03	0.41
1:F:191:HIS:HB2	1:F:274:TRP:NE1	2.35	0.41
4:I:101:VAL:HG22	4:I:122:LYS:HD2	2.02	0.40
4:D:149:VAL:HG12	4:D:192:TRP:HB3	2.03	0.40
5:E:72:GLU:HB2	5:E:75:LYS:HB2	2.02	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	275/276 (100%)	265 (96%)	9 (3%)	1 (0%)	34 60
1	F	275/276 (100%)	262 (95%)	12 (4%)	1 (0%)	34 60

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	B	97/100 (97%)	95 (98%)	2 (2%)	0	100 100
2	G	97/100 (97%)	96 (99%)	1 (1%)	0	100 100
3	C	7/9 (78%)	7 (100%)	0	0	100 100
3	H	7/9 (78%)	7 (100%)	0	0	100 100
4	D	203/205 (99%)	195 (96%)	8 (4%)	0	100 100
4	I	203/205 (99%)	191 (94%)	12 (6%)	0	100 100
5	E	243/245 (99%)	232 (96%)	10 (4%)	1 (0%)	34 60
5	J	243/245 (99%)	224 (92%)	18 (7%)	1 (0%)	34 60
All	All	1650/1670 (99%)	1574 (95%)	72 (4%)	4 (0%)	47 73

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	J	148	ILE
1	A	251	SER
5	E	166	ASP
1	F	251	SER

### 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	235/234 (100%)	224 (95%)	11 (5%)	26 54
1	F	235/234 (100%)	222 (94%)	13 (6%)	21 46
2	B	94/95 (99%)	90 (96%)	4 (4%)	29 57
2	G	94/95 (99%)	88 (94%)	6 (6%)	17 39
3	C	9/9 (100%)	9 (100%)	0	100 100
3	H	9/9 (100%)	9 (100%)	0	100 100
4	D	182/182 (100%)	169 (93%)	13 (7%)	14 34
4	I	182/182 (100%)	170 (93%)	12 (7%)	16 38

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
5	E	216/216 (100%)	196 (91%)	20 (9%)	9 21
5	J	216/216 (100%)	189 (88%)	27 (12%)	4 10
All	All	1472/1472 (100%)	1366 (93%)	106 (7%)	14 34

All (106) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	ARG
1	A	39	ASP
1	A	61	ASP
1	A	73	THR
1	A	76	GLU
1	A	88	SER
1	A	110	LEU
1	A	156	LEU
1	A	197	HIS
1	A	225	THR
1	A	230	LEU
2	B	39	LEU
2	B	48	LYS
2	B	70	PHE
2	B	88	SER
4	D	0	MET
4	D	12	SER
4	D	27	ASP
4	D	46	LEU
4	D	76	ILE
4	D	89	LEU
4	D	140	ARG
4	D	145	SER
4	D	146	ASP
4	D	156	ASP
4	D	158	GLN
4	D	183	ASP
4	D	215	PHE
5	E	3	VAL
5	E	19	VAL
5	E	48	GLN
5	E	64	LYS
5	E	73	LYS
5	E	85	THR

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Mol	Chain	Res	Type
5	E	89	LEU
5	E	145	GLU
5	E	156	LEU
5	E	166	ASP
5	E	168	VAL
5	E	177	LYS
5	E	184	CYS
5	E	193	GLN
5	E	196	LEU
5	E	198	ASP
5	E	215	GLN
5	E	239	ASP
5	E	240	ARG
5	E	253	TRP
1	F	35	ARG
1	F	65	GLN
1	F	73	THR
1	F	75	ARG
1	F	88	SER
1	F	103	LEU
1	F	110	LEU
1	F	145	ARG
1	F	156	LEU
1	F	157	ARG
1	F	183	ASP
1	F	197	HIS
1	F	230	LEU
2	G	19	LYS
2	G	39	LEU
2	G	48	LYS
2	G	70	PHE
2	G	75	LYS
2	G	88	SER
4	I	0	MET
4	I	12	SER
4	I	27	ASP
4	I	37	ASN
4	I	46	LEU
4	I	76	ILE
4	I	89	LEU
4	I	141	ASP
4	I	158	GLN

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Mol	Chain	Res	Type
4	I	168	ASP
4	I	176	VAL
4	I	205	ASN
5	J	3	VAL
5	J	19	VAL
5	J	47	LYS
5	J	48	GLN
5	J	64	LYS
5	J	72	GLU
5	J	73	LYS
5	J	75	LYS
5	J	85	THR
5	J	89	LEU
5	J	123	ARG
5	J	147	GLU
5	J	148	ILE
5	J	158	CYS
5	J	159	LEU
5	J	161	THR
5	J	168	VAL
5	J	175	ASN
5	J	183	VAL
5	J	184	CYS
5	J	196	LEU
5	J	220	HIS
5	J	223	CYS
5	J	239	ASP
5	J	240	ARG
5	J	249	SER
5	J	253	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
4	D	202	ASN
5	E	48	GLN
5	E	215	GLN
5	J	175	ASN
5	J	220	HIS
5	J	224	GLN

### 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 monosaccharides 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 (i)

### 6.1 Protein, DNA and RNA chains (i)

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%)	0.63	47 (17%) 1 1	29, 68, 177, 207	7 (2%)
1	F	276/276 (100%)	0.36	39 (14%) 2 1	21, 52, 185, 205	8 (2%)
2	B	99/100 (99%)	0.65	11 (11%) 5 4	47, 90, 127, 138	6 (6%)
2	G	99/100 (99%)	0.00	1 (1%) 82 83	32, 62, 100, 115	6 (6%)
3	C	9/9 (100%)	0.09	0 100 100	29, 34, 43, 50	0
3	H	9/9 (100%)	0.25	0 100 100	26, 32, 36, 39	0
4	D	205/205 (100%)	0.06	8 (3%) 39 38	32, 61, 105, 139	1 (0%)
4	I	205/205 (100%)	1.88	64 (31%) 0 0	32, 91, 226, 253	0
5	E	245/245 (100%)	0.12	13 (5%) 26 25	27, 57, 103, 144	0
5	J	245/245 (100%)	1.89	79 (32%) 0 0	27, 107, 230, 263	0
All	All	1668/1670 (99%)	0.74	262 (15%) 2 1	21, 67, 193, 263	28 (1%)

All (262) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	J	257	ASP	21.5
4	I	206	ASN	17.5
5	J	256	ALA	16.4
4	I	218	PRO	14.1
5	J	216	ASN	14.0
4	I	198	PHE	13.0
5	J	219	ASN	12.2
5	J	211	ALA	11.8
5	J	251	GLU	11.6
5	J	212	THR	11.1
4	I	140	ARG	10.7
5	J	253	TRP	10.1
5	J	210	SER	9.9

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Mol	Chain	Res	Type	RSRZ
4	I	205	ASN	9.7
5	J	155	THR	9.6
4	I	145	SER	9.4
4	I	180	ARG	9.3
4	I	209	ILE	9.2
5	J	206	ARG	9.0
5	J	178	GLU	8.6
4	I	207	SER	8.5
4	I	156	ASP	8.4
1	A	193	PRO	8.1
4	I	217	SER	7.9
4	I	216	PRO	7.9
5	J	180	HIS	7.8
5	J	239	ASP	7.8
4	I	142	SER	7.8
5	J	217	PRO	7.7
4	I	136	VAL	7.6
5	J	157	VAL	7.6
1	F	1	GLY	7.6
5	J	249	SER	7.6
1	A	258	THR	7.5
5	J	213	PHE	7.5
4	I	196	SER	7.4
4	I	204	PHE	7.4
1	F	194	VAL	7.2
5	J	149	SER	7.1
1	A	194	VAL	7.0
4	I	141	ASP	7.0
1	A	199	ALA	6.8
4	I	130	GLN	6.8
5	J	175	ASN	6.8
2	B	1	ILE	6.8
5	J	208	ARG	6.7
5	J	148	ILE	6.7
5	J	174	VAL	6.6
5	J	176	GLY	6.6
4	I	194	ASN	6.5
4	I	211	GLU	6.4
5	J	242	LYS	6.4
1	F	226	GLN	6.3
5	J	177	LYS	6.3
5	J	207	LEU	6.2

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Mol	Chain	Res	Type	RSRZ
5	J	141	PHE	6.2
1	A	273	ARG	6.2
5	J	156	LEU	6.0
5	J	224	GLN	6.0
4	I	212	ASP	5.9
5	J	142	GLU	5.9
1	A	257	TYR	5.9
5	J	152	GLN	5.9
5	J	252	ALA	5.9
5	J	171	SER	5.7
5	J	214	TRP	5.7
5	J	241	ALA	5.6
2	G	1	ILE	5.5
4	I	178	ASP	5.5
5	J	205	SER	5.5
5	J	218	ARG	5.4
1	F	196	ASP	5.4
4	I	169	VAL	5.3
4	I	183	ASP	5.3
4	I	199	ALA	5.3
4	I	210	PRO	5.3
5	J	179	VAL	5.1
5	J	196	LEU	5.1
1	A	195	SER	5.0
5	J	158	CYS	5.0
1	F	274	TRP	5.0
4	I	137	TYR	5.0
4	I	138	GLN	5.0
4	I	193	SER	4.9
4	I	143	LYS	4.9
1	F	220	ASP	4.9
5	J	153	LYS	4.9
1	F	198	GLU	4.8
5	J	181	SER	4.8
1	F	225	THR	4.7
4	I	168	ASP	4.7
5	E	257	ASP	4.7
1	A	276	PRO	4.7
5	J	140	VAL	4.7
1	F	197	HIS	4.6
4	I	213	THR	4.6
1	A	248	VAL	4.6

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Mol	Chain	Res	Type	RSRZ
4	D	180	ARG	4.6
4	I	149	VAL	4.5
1	A	105	PRO	4.5
1	A	219	ARG	4.5
4	I	208	ILE	4.4
4	I	197	ASP	4.4
5	J	173	TRP	4.4
4	D	196	SER	4.3
1	F	191	HIS	4.3
5	J	223	CYS	4.3
2	B	99	MET	4.2
4	I	166	ASP	4.2
1	F	219	ARG	4.2
1	F	222	GLU	4.2
1	F	195	SER	4.1
1	F	250	PRO	4.1
1	A	108	ARG	4.0
1	F	192	HIS	4.0
4	I	131	ASN	4.0
5	J	151	THR	4.0
1	A	197	HIS	3.9
4	I	164	SER	3.9
5	J	254	GLY	3.9
5	J	221	PHE	3.9
4	I	150	CYS	3.8
1	A	246	ALA	3.8
5	J	250	ALA	3.8
1	F	252	GLY	3.8
4	I	144	SER	3.8
1	F	253	GLU	3.8
4	I	135	ALA	3.7
1	F	260	HIS	3.7
4	I	189	ALA	3.7
1	F	251	SER	3.7
1	A	260	HIS	3.6
5	J	233	ASN	3.6
5	J	139	ALA	3.5
1	F	273	ARG	3.5
1	A	252	GLY	3.5
5	J	154	ALA	3.5
1	F	248	VAL	3.5
5	J	183	VAL	3.5

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Mol	Chain	Res	Type	RSRZ
5	J	236	TRP	3.5
1	A	227	ASP	3.4
1	A	247	VAL	3.4
4	I	185	LYS	3.4
5	J	195	ALA	3.4
5	J	143	PRO	3.4
1	A	41	ALA	3.4
5	J	209	VAL	3.4
4	I	165	LYS	3.4
5	J	172	TRP	3.4
1	A	256	ARG	3.4
5	J	150	HIS	3.3
1	A	201	LEU	3.3
1	A	274	TRP	3.2
5	J	48	GLN	3.2
1	F	199	ALA	3.2
4	I	177	LEU	3.2
1	F	270	LEU	3.2
1	A	42	SER	3.2
4	I	195	LYS	3.1
4	I	133	ASP	3.1
5	J	47	LYS	3.1
1	F	189	VAL	3.1
5	E	232	GLU	3.1
1	F	223	ASP	3.1
5	J	247	ILE	3.0
4	I	214	PHE	3.0
4	I	181	SER	3.0
4	I	152	PHE	3.0
4	I	190	VAL	3.0
5	J	182	GLY	3.0
1	A	218	GLN	3.0
1	A	217	TRP	2.9
5	J	255	ARG	2.9
1	F	41	ALA	2.9
1	A	253	GLU	2.9
1	F	249	VAL	2.9
4	D	197	ASP	2.9
4	I	148	SER	2.9
4	I	139	LEU	2.8
4	I	163	GLN	2.8
2	B	45	ARG	2.8

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Mol	Chain	Res	Type	RSRZ
5	E	46	PRO	2.8
4	I	167	SER	2.8
1	A	272	LEU	2.8
5	J	191	LYS	2.8
1	A	264	GLU	2.8
5	E	196	LEU	2.8
5	J	244	VAL	2.8
5	E	195	ALA	2.7
5	J	198	ASP	2.7
1	F	257	TYR	2.7
1	F	276	PRO	2.7
4	I	146	ASP	2.7
1	A	1	GLY	2.7
1	A	249	VAL	2.7
5	J	59	GLY	2.7
4	I	192	TRP	2.7
4	I	147	LYS	2.7
4	D	218	PRO	2.6
5	E	215	GLN	2.6
5	J	226	GLN	2.6
4	D	0	MET	2.6
1	A	17	ARG	2.6
1	A	261	VAL	2.6
1	A	222	GLU	2.6
1	A	181	ARG	2.6
1	A	183	ASP	2.6
2	B	16	GLU	2.6
4	I	182	MET	2.6
1	A	262	GLN	2.5
5	E	233	ASN	2.5
1	A	223	ASP	2.5
5	J	240	ARG	2.5
2	B	89	GLN	2.5
1	A	177	GLU	2.5
1	F	187	THR	2.5
4	D	145	SER	2.5
2	B	2	GLN	2.5
5	E	256	ALA	2.5
5	J	235	GLU	2.5
2	B	69	GLU	2.4
5	J	228	TYR	2.4
5	J	197	ASN	2.4

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Mol	Chain	Res	Type	RSRZ
2	B	43	GLY	2.4
1	F	271	THR	2.4
5	J	193	GLN	2.4
1	F	218	GLN	2.3
1	F	201	LEU	2.3
4	I	151	LEU	2.3
1	F	200	THR	2.3
1	A	192	HIS	2.3
4	I	191	ALA	2.3
1	A	250	PRO	2.3
4	I	188	SER	2.3
5	E	241	ALA	2.2
1	A	275	GLU	2.2
5	E	242	LYS	2.2
2	B	46	ILE	2.2
5	J	232	GLU	2.2
4	I	157	SER	2.2
1	F	193	PRO	2.2
1	A	255	GLN	2.2
5	J	245	THR	2.2
2	B	17	ASN	2.2
5	J	147	GLU	2.2
1	F	256	ARG	2.2
1	F	182	ALA	2.1
4	I	215	PHE	2.1
4	D	158	GLN	2.1
5	E	155	THR	2.1
2	B	77	GLU	2.1
1	A	44	ARG	2.1
4	D	182	MET	2.1
1	A	220	ASP	2.1
5	E	239	ASP	2.1
1	A	191	HIS	2.1
1	A	182	ALA	2.1
1	F	246	ALA	2.1
1	F	181	ARG	2.1
1	A	200	THR	2.1
5	J	248	VAL	2.0
5	E	235	GLU	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 monosaccharides 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.