



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 16, 2021 – 11:50 PM EDT

PDB ID : 1S7R  
Title : Crystal structures of the murine class I major histocompatibility complex H-2Kb in complex with LCMV-derived gp33 index peptide and three of its escape variants  
Authors : Velloso, L.M.; Michaelsson, J.; Ljunggren, H.G.; Schneider, G.; Achour, A.  
Deposited on : 2004-01-30  
Resolution : 2.95 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

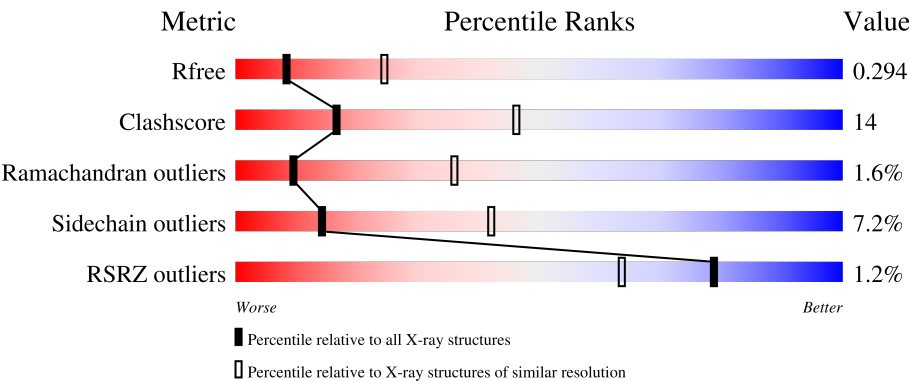
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:  
*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.95 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 <sub>free</sub>	130704	3104 (3.00-2.92)
Clashscore	141614	3462 (3.00-2.92)
Ramachandran outliers	138981	3340 (3.00-2.92)
Sidechain outliers	138945	3343 (3.00-2.92)
RSRZ outliers	127900	2986 (3.00-2.92)

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	348	<div><div></div><div>51%26%•21%</div></div>
1	D	348	<div><div>2%</div><div>53%24%•21%</div></div>
2	B	99	<div><div></div><div>64%31%5%</div></div>
2	E	99	<div><div></div><div>63%32%5%</div></div>
3	C	9	<div><div>11%</div><div>22%78%</div></div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	F	9	<div> <div>11%</div> <div>33%</div> <div>67%</div> </div>

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 6339 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 H-2 class I histocompatibility antigen, K-B alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	276	Total	C	N	O	S	0	0	0
			2247	1418	395	425	9			
1	D	276	Total	C	N	O	S	0	0	0
			2247	1418	395	425	9			

- 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
			821	524	138	152	7			
2	E	99	Total	C	N	O	S	0	0	0
			821	524	138	152	7			

- Molecule 3 is a protein called Glycoprotein 9-residue peptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	9	Total	C	N	O	S	0	0	0
			70	45	11	13	1			
3	F	9	Total	C	N	O	S	0	0	0
			70	45	11	13	1			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	6	LEU	PHE	engineered mutation	UNP P07399
C	9	MET	CYS	SEE REMARK 999	UNP P07399
F	6	LEU	PHE	engineered mutation	UNP P07399
F	9	MET	CYS	SEE REMARK 999	UNP P07399

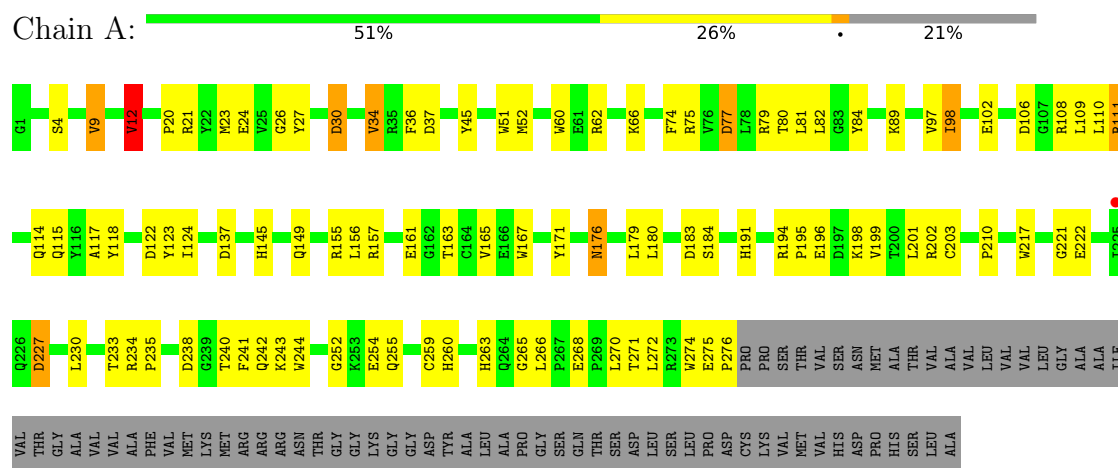
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	21	Total 21	O 21	0	0
4	B	10	Total 10	O 10	0	0
4	D	24	Total 24	O 24	0	0
4	E	8	Total 8	O 8	0	0

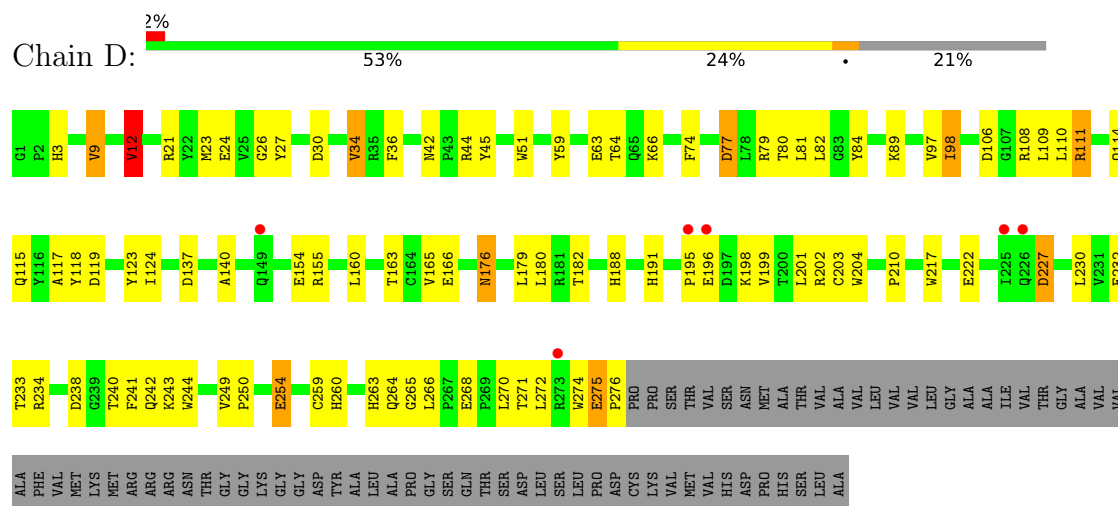
### 3 Residue-property plots

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: H-2 class I histocompatibility antigen, K-B alpha chain



- Molecule 1: H-2 class I histocompatibility antigen, K-B alpha chain



- Molecule 2: Beta-2-microglobulin





- Molecule 2: Beta-2-microglobulin



- Molecule 3: Glycoprotein 9-residue peptide



- Molecule 3: Glycoprotein 9-residue peptide



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	50.19Å 88.52Å 120.03Å 90.00° 94.00° 90.00°	Depositor
Resolution (Å)	24.84 – 2.95 24.80 – 2.95	Depositor EDS
% Data completeness (in resolution range)	93.4 (24.84-2.95) 93.4 (24.80-2.95)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.41 (at 2.94Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, $R_{free}$	0.239 , 0.290 0.242 , 0.294	Depositor DCC
$R_{free}$ test set	1041 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	42.5	Xtriage
Anisotropy	0.153	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 30.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.86	EDS
Total number of atoms	6339	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 21.95 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 6.3039e-03.*

<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	0.76	0/2309	0.88	8/3137 (0.3%)
1	D	0.64	0/2309	0.83	5/3137 (0.2%)
2	B	0.77	0/847	0.88	3/1148 (0.3%)
2	E	0.59	0/847	0.83	1/1148 (0.1%)
3	C	0.72	0/70	1.03	0/92
3	F	0.57	0/70	0.93	0/92
All	All	0.70	0/6452	0.86	17/8754 (0.2%)

There are no bond length outliers.

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	77	ASP	CB-CG-OD2	6.28	123.95	118.30
1	A	122	ASP	CB-CG-OD2	6.27	123.94	118.30
1	A	137	ASP	CB-CG-OD2	6.25	123.93	118.30
1	A	106	ASP	CB-CG-OD2	5.99	123.69	118.30
2	B	59	ASP	CB-CG-OD2	5.82	123.54	118.30
1	D	106	ASP	CB-CG-OD2	5.52	123.26	118.30
1	D	227	ASP	CB-CG-OD2	5.43	123.19	118.30
1	A	227	ASP	CB-CG-OD2	5.41	123.17	118.30
1	A	37	ASP	CB-CG-OD2	5.39	123.15	118.30
2	E	85	ASP	CB-CG-OD2	5.33	123.10	118.30
1	D	119	ASP	CB-CG-OD2	5.24	123.02	118.30
1	A	30	ASP	CB-CG-OD2	5.23	123.01	118.30
2	B	98	ASP	CB-CG-OD2	5.15	122.94	118.30
1	D	77	ASP	CB-CG-OD2	5.15	122.94	118.30
1	A	183	ASP	CB-CG-OD2	5.09	122.88	118.30
1	D	137	ASP	CB-CG-OD2	5.06	122.85	118.30
2	B	85	ASP	CB-CG-OD2	5.01	122.81	118.30

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	A	2247	0	2136	67	0
1	D	2247	0	2136	64	0
2	B	821	0	796	22	0
2	E	821	0	796	26	0
3	C	70	0	76	9	0
3	F	70	0	76	6	0
4	A	21	0	0	3	0
4	B	10	0	0	0	0
4	D	24	0	0	3	0
4	E	8	0	0	2	0
All	All	6339	0	6016	174	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 14.

All (174) 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:191:HIS:NE2	1:A:254:GLU:OE2	1.94	0.98
1:D:191:HIS:NE2	1:D:254:GLU:OE2	2.03	0.91
2:E:41:LYS:HB2	2:E:46:ILE:HD11	1.68	0.76
2:B:41:LYS:HB2	2:B:46:ILE:HD11	1.70	0.73
1:D:176:ASN:HD22	1:D:180:LEU:HD12	1.57	0.69
1:D:195:PRO:O	1:D:196:GLU:HB3	1.95	0.67
1:D:27:TYR:OH	2:E:53:ASP:HA	1.95	0.67
1:A:195:PRO:O	1:A:196:GLU:HB3	1.95	0.66
2:B:10:TYR:O	2:B:24:ASN:HB2	1.98	0.64
1:D:82:LEU:HD13	1:D:89:LYS:HD3	1.78	0.64
1:A:167:TRP:HE1	3:C:1:LYS:HB3	1.62	0.63
1:A:82:LEU:HD13	1:A:89:LYS:HD3	1.81	0.62
2:E:10:TYR:O	2:E:24:ASN:HB2	1.99	0.62
1:D:233:THR:OG1	1:D:243:LYS:HE2	1.99	0.62
1:A:263:HIS:CD2	1:A:265:GLY:H	2.18	0.62
1:D:238:ASP:OD1	1:D:240:THR:HG23	2.00	0.61
1:A:194:ARG:O	4:A:364:HOH:O	2.16	0.61

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:242:GLN:OE1	2:E:10:TYR:CD1	2.54	0.61
1:A:221:GLY:HA3	4:A:358:HOH:O	2.01	0.60
2:E:21:ASN:HB3	2:E:70:PHE:CE1	2.37	0.60
1:D:274:TRP:O	1:D:276:PRO:HD3	2.02	0.60
1:D:9:VAL:HB	1:D:24:GLU:HG2	1.84	0.59
1:D:210:PRO:O	1:D:263:HIS:HE1	1.86	0.59
1:A:157:ARG:HG2	1:A:161:GLU:HG3	1.84	0.58
2:B:59:ASP:O	2:B:60:TRP:HB2	2.03	0.58
1:A:27:TYR:OH	2:B:53:ASP:HA	2.03	0.58
2:B:21:ASN:HB3	2:B:70:PHE:CE1	2.39	0.57
1:A:238:ASP:OD1	1:A:240:THR:HG23	2.04	0.57
1:D:155:ARG:HD3	3:F:4:TYR:OH	2.05	0.57
1:A:9:VAL:HB	1:A:24:GLU:HG2	1.85	0.57
1:D:202:ARG:HD3	1:D:244:TRP:CD2	2.39	0.57
1:A:81:LEU:HD12	1:A:84:TYR:CD2	2.39	0.57
1:A:81:LEU:HD12	1:A:84:TYR:HD2	1.69	0.56
2:E:59:ASP:O	2:E:60:TRP:HB2	2.05	0.56
1:A:30:ASP:HB3	1:A:241:PHE:CZ	2.40	0.56
1:A:210:PRO:O	1:A:263:HIS:HE1	1.89	0.56
1:A:98:ILE:HG22	1:A:115:GLN:HB2	1.88	0.56
1:A:80:THR:HG22	1:A:84:TYR:CE2	2.41	0.55
2:B:41:LYS:CB	2:B:46:ILE:HD11	2.36	0.55
1:D:12:VAL:HG13	1:D:21:ARG:HB3	1.88	0.54
1:A:260:HIS:CE1	1:A:271:THR:HG23	2.42	0.54
1:D:201:LEU:HD11	1:D:254:GLU:HB2	1.89	0.54
1:A:233:THR:OG1	1:A:243:LYS:HE2	2.08	0.54
1:D:30:ASP:HB3	1:D:241:PHE:CZ	2.42	0.54
1:A:201:LEU:HD11	1:A:254:GLU:HB2	1.90	0.54
1:D:42:ASN:HB3	4:D:367:HOH:O	2.07	0.54
1:D:26:GLY:HA3	1:D:34:VAL:HG23	1.90	0.54
4:D:355:HOH:O	2:E:99:MET:HE1	2.08	0.53
2:E:41:LYS:CB	2:E:46:ILE:HD11	2.36	0.53
1:D:80:THR:HG22	1:D:84:TYR:CE2	2.43	0.53
1:D:263:HIS:CD2	1:D:265:GLY:H	2.26	0.53
1:A:26:GLY:HA3	1:A:34:VAL:HG23	1.89	0.53
1:A:123:TYR:HD2	1:A:124:ILE:HG22	1.74	0.53
1:D:97:VAL:HA	1:D:115:GLN:O	2.09	0.53
1:A:12:VAL:HG13	1:A:21:ARG:HB3	1.91	0.53
1:D:23:MET:HG3	1:D:36:PHE:O	2.07	0.53
1:A:51:TRP:CH2	1:A:179:LEU:HD11	2.44	0.52
1:D:202:ARG:HD3	1:D:244:TRP:CG	2.43	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:81:LEU:HD12	1:D:84:TYR:CD2	2.44	0.52
2:E:3:LYS:NZ	2:E:59:ASP:OD2	2.42	0.52
1:A:260:HIS:HA	1:A:270:LEU:O	2.10	0.52
2:E:40:LEU:HD23	2:E:45:LYS:HA	1.92	0.52
1:A:74:PHE:HA	1:A:77:ASP:HB2	1.91	0.52
1:A:155:ARG:HD3	3:C:4:TYR:OH	2.10	0.51
1:A:77:ASP:HB3	3:C:9:MET:HE3	1.92	0.51
1:D:160:LEU:O	1:D:165:VAL:HG13	2.10	0.51
1:D:81:LEU:HD12	1:D:84:TYR:HD2	1.75	0.51
1:A:167:TRP:NE1	3:C:1:LYS:HB3	2.26	0.51
1:A:274:TRP:O	1:A:276:PRO:HD3	2.11	0.51
2:B:40:LEU:HA	2:B:44:LYS:O	2.09	0.51
1:D:74:PHE:HA	1:D:77:ASP:HB2	1.91	0.51
1:D:176:ASN:HD22	1:D:180:LEU:CD1	2.23	0.50
2:B:3:LYS:NZ	2:B:59:ASP:OD2	2.44	0.50
2:B:7:ILE:CD1	2:B:82:VAL:HB	2.42	0.50
2:E:7:ILE:CD1	2:E:82:VAL:HB	2.41	0.50
1:A:167:TRP:O	1:A:171:TYR:CD2	2.63	0.50
1:A:196:GLU:O	1:A:196:GLU:HG2	2.11	0.50
2:B:40:LEU:HD23	2:B:45:LYS:HA	1.93	0.50
1:D:98:ILE:HG22	1:D:115:GLN:HB2	1.93	0.50
1:D:123:TYR:HD2	1:D:124:ILE:HG22	1.76	0.49
2:B:6:GLN:HG3	2:B:29:GLN:OE1	2.11	0.49
1:D:109:LEU:HD13	1:D:165:VAL:CG1	2.43	0.49
2:E:3:LYS:NZ	2:E:59:ASP:OD1	2.45	0.49
1:A:259:CYS:O	1:A:271:THR:HA	2.13	0.49
1:D:259:CYS:O	1:D:271:THR:HA	2.13	0.49
1:D:266:LEU:HD13	1:D:270:LEU:HG	1.94	0.49
1:D:24:GLU:HB2	1:D:36:PHE:HB3	1.96	0.48
1:A:23:MET:HG3	1:A:36:PHE:O	2.13	0.48
1:A:202:ARG:HD3	1:A:244:TRP:CD2	2.49	0.47
1:D:232:GLU:OE1	2:E:29:GLN:NE2	2.46	0.47
1:D:260:HIS:HA	1:D:270:LEU:O	2.13	0.47
1:A:74:PHE:CE2	3:C:6:LEU:HD13	2.48	0.47
1:A:79:ARG:O	1:A:82:LEU:HB2	2.14	0.47
3:C:3:VAL:HG22	3:C:4:TYR:N	2.29	0.47
2:B:15:PRO:HG3	2:B:95:TRP:HZ2	1.79	0.47
1:D:51:TRP:CH2	1:D:179:LEU:HD11	2.50	0.46
1:D:117:ALA:HB2	2:E:60:TRP:CE2	2.51	0.46
1:A:266:LEU:HD13	1:A:270:LEU:HG	1.96	0.46
1:D:234:ARG:O	1:D:241:PHE:HA	2.16	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:20:PRO:HD2	1:A:75:ARG:HD2	1.97	0.46
1:A:117:ALA:HB2	2:B:60:TRP:CE2	2.50	0.46
1:D:203:CYS:HB2	1:D:217:TRP:CZ2	2.50	0.46
1:D:260:HIS:CE1	1:D:271:THR:HG23	2.51	0.46
1:A:74:PHE:CZ	3:C:6:LEU:HD13	2.51	0.46
1:D:3:HIS:NE2	1:D:180:LEU:HD21	2.31	0.46
1:A:97:VAL:HA	1:A:115:GLN:O	2.15	0.46
1:A:108:ARG:HH11	1:A:108:ARG:HG2	1.81	0.46
1:D:195:PRO:O	1:D:196:GLU:CB	2.62	0.46
4:A:355:HOH:O	2:B:99:MET:HE1	2.15	0.46
1:D:98:ILE:O	1:D:114:GLN:HA	2.17	0.45
2:E:15:PRO:HG3	2:E:95:TRP:HZ2	1.80	0.45
3:F:3:VAL:HG22	3:F:4:TYR:N	2.31	0.45
1:A:98:ILE:O	1:A:114:GLN:HA	2.17	0.45
1:A:252:GLY:O	1:A:255:GLN:NE2	2.45	0.45
2:E:12:ARG:NH1	2:E:13:HIS:CE1	2.84	0.45
2:E:52:SER:OG	2:E:65:LEU:HD23	2.17	0.45
2:B:3:LYS:NZ	2:B:59:ASP:OD1	2.49	0.44
1:A:202:ARG:HD3	1:A:244:TRP:CG	2.52	0.44
1:A:110:LEU:O	1:A:111:ARG:HB2	2.17	0.44
2:E:40:LEU:HA	2:E:44:LYS:O	2.18	0.44
1:A:242:GLN:OE1	2:B:10:TYR:CD1	2.70	0.44
1:D:191:HIS:NE2	1:D:199:VAL:HG11	2.33	0.44
1:A:24:GLU:HB2	1:A:36:PHE:HB3	1.99	0.44
1:D:79:ARG:O	1:D:82:LEU:HB2	2.17	0.44
1:D:81:LEU:HD23	1:D:118:TYR:CD1	2.52	0.44
1:D:249:VAL:HB	1:D:250:PRO:HD2	2.00	0.43
1:A:234:ARG:O	1:A:241:PHE:HA	2.18	0.43
1:D:108:ARG:HG2	1:D:108:ARG:HH11	1.82	0.43
2:E:49:VAL:HG22	2:E:68:THR:HB	1.99	0.43
1:A:81:LEU:HD23	1:A:118:TYR:CD1	2.53	0.43
1:D:63:GLU:OE1	3:F:3:VAL:HG12	2.18	0.43
1:A:195:PRO:O	1:A:196:GLU:CB	2.62	0.43
2:E:27:VAL:HG11	2:E:35:ILE:CD1	2.48	0.43
1:A:108:ARG:HG2	1:A:108:ARG:NH1	2.34	0.43
1:A:176:ASN:O	1:A:180:LEU:HB2	2.18	0.43
1:A:191:HIS:NE2	1:A:199:VAL:HG11	2.33	0.43
1:D:110:LEU:O	1:D:111:ARG:HB2	2.19	0.43
1:D:196:GLU:HG2	1:D:196:GLU:O	2.19	0.43
2:E:85:ASP:HB3	4:E:100:HOH:O	2.18	0.43
1:A:203:CYS:HB2	1:A:217:TRP:CZ2	2.53	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:81:LEU:HD23	1:D:118:TYR:CG	2.54	0.43
2:E:7:ILE:HB	2:E:93:VAL:HG21	2.00	0.42
1:A:62:ARG:O	1:A:66:LYS:HG2	2.19	0.42
1:A:109:LEU:HD13	1:A:165:VAL:CG1	2.49	0.42
1:D:77:ASP:HB3	3:F:9:MET:HE3	2.00	0.42
2:B:36:GLU:O	2:B:82:VAL:HA	2.20	0.42
1:D:59:TYR:HB2	4:D:354:HOH:O	2.19	0.42
1:A:51:TRP:CZ2	1:A:179:LEU:HD11	2.55	0.42
1:A:98:ILE:O	1:A:98:ILE:CG2	2.67	0.42
2:E:12:ARG:HD2	2:E:12:ARG:C	2.40	0.42
1:A:81:LEU:HD23	1:A:118:TYR:CG	2.54	0.42
1:D:74:PHE:CE2	3:F:6:LEU:HD13	2.55	0.42
1:D:188:HIS:CE1	1:D:204:TRP:HB2	2.54	0.42
1:D:66:LYS:HE2	3:F:3:VAL:HG13	2.02	0.42
1:A:4:SER:HB3	1:A:102:GLU:HB3	2.02	0.41
1:A:167:TRP:NE1	3:C:1:LYS:O	2.53	0.41
1:D:182:THR:HG21	1:D:264:GLN:HB3	2.02	0.41
1:A:52:MET:O	1:A:60:TRP:HZ2	2.03	0.41
1:D:123:TYR:CZ	1:D:140:ALA:HA	2.56	0.41
2:E:7:ILE:HD11	2:E:82:VAL:HB	2.02	0.41
1:A:234:ARG:HA	1:A:235:PRO:HD3	1.90	0.41
2:B:49:VAL:HG22	2:B:68:THR:HB	2.03	0.41
1:D:274:TRP:CD1	1:D:275:GLU:N	2.89	0.41
1:A:145:HIS:O	1:A:149:GLN:HG2	2.21	0.41
2:B:52:SER:OG	2:B:65:LEU:HD23	2.20	0.41
1:D:44:ARG:HA	1:D:64:THR:HG23	2.03	0.41
1:D:108:ARG:HG2	1:D:108:ARG:NH1	2.36	0.41
2:E:85:ASP:CB	4:E:100:HOH:O	2.68	0.41
1:A:66:LYS:HE2	3:C:3:VAL:HG13	2.03	0.40
2:B:12:ARG:HD2	2:B:12:ARG:C	2.41	0.40
2:B:19:LYS:HA	2:B:20:PRO:HD3	1.91	0.40
2:B:7:ILE:HD11	2:B:82:VAL:HB	2.03	0.40
1:D:165:VAL:HG23	1:D:166:GLU:HG3	2.02	0.40
2:E:31:HIS:ND1	2:E:32:PRO:HA	2.37	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	274/348 (79%)	248 (90%)	23 (8%)	3 (1%)	14	46
1	D	274/348 (79%)	246 (90%)	25 (9%)	3 (1%)	14	46
2	B	97/99 (98%)	93 (96%)	2 (2%)	2 (2%)	7	29
2	E	97/99 (98%)	93 (96%)	2 (2%)	2 (2%)	7	29
3	C	7/9 (78%)	5 (71%)	1 (14%)	1 (14%)	0	1
3	F	7/9 (78%)	5 (71%)	1 (14%)	1 (14%)	0	1
All	All	756/912 (83%)	690 (91%)	54 (7%)	12 (2%)	9	36

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	88	ALA
2	E	60	TRP
2	E	88	ALA
3	F	2	ALA
1	D	111	ARG
1	A	12	VAL
1	A	111	ARG
2	B	60	TRP
3	C	2	ALA
1	D	12	VAL
1	A	275	GLU
1	D	275	GLU

### 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	234/290 (81%)	219 (94%)	15 (6%)	17	47
1	D	234/290 (81%)	219 (94%)	15 (6%)	17	47
2	B	94/94 (100%)	86 (92%)	8 (8%)	10	34
2	E	94/94 (100%)	86 (92%)	8 (8%)	10	34
3	C	7/7 (100%)	6 (86%)	1 (14%)	3	13
3	F	7/7 (100%)	6 (86%)	1 (14%)	3	13
All	All	670/782 (86%)	622 (93%)	48 (7%)	14	42

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	VAL
1	A	12	VAL
1	A	34	VAL
1	A	45	TYR
1	A	98	ILE
1	A	156	LEU
1	A	163	THR
1	A	176	ASN
1	A	184	SER
1	A	198	LYS
1	A	222	GLU
1	A	227	ASP
1	A	230	LEU
1	A	268	GLU
1	A	272	LEU
2	B	12	ARG
2	B	29	GLN
2	B	48	LYS
2	B	56	PHE
2	B	57	SER
2	B	64	ILE
2	B	70	PHE
2	B	89	GLU
3	C	8	THR
1	D	9	VAL
1	D	12	VAL
1	D	34	VAL
1	D	45	TYR

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	D	98	ILE
1	D	154	GLU
1	D	163	THR
1	D	176	ASN
1	D	198	LYS
1	D	222	GLU
1	D	227	ASP
1	D	230	LEU
1	D	254	GLU
1	D	268	GLU
1	D	272	LEU
2	E	12	ARG
2	E	29	GLN
2	E	48	LYS
2	E	56	PHE
2	E	64	ILE
2	E	70	PHE
2	E	89	GLU
2	E	97	ARG
3	F	8	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	176	ASN
1	A	188	HIS
1	A	220	ASN
1	A	263	HIS
1	A	264	GLN
2	B	2	GLN
2	B	13	HIS
2	B	38	GLN
1	D	176	ASN
1	D	188	HIS
1	D	220	ASN
1	D	263	HIS
1	D	264	GLN
2	E	2	GLN
2	E	13	HIS

### 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	276/348 (79%)	-0.34	1 (0%) 92 84	6, 23, 43, 57	0
1	D	276/348 (79%)	-0.09	6 (2%) 62 45	6, 23, 43, 57	0
2	B	99/99 (100%)	-0.46	0 100 100	8, 20, 34, 38	0
2	E	99/99 (100%)	-0.20	0 100 100	8, 20, 34, 38	0
3	C	9/9 (100%)	0.40	1 (11%) 5 3	39, 40, 41, 42	0
3	F	9/9 (100%)	0.45	1 (11%) 5 3	39, 40, 42, 42	0
All	All	768/912 (84%)	-0.23	9 (1%) 79 63	6, 23, 42, 57	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	225	ILE	3.5
1	D	196	GLU	2.9
1	D	225	ILE	2.9
1	D	226	GLN	2.7
1	D	273	ARG	2.3
1	D	195	PRO	2.2
1	D	149	GLN	2.2
3	F	2	ALA	2.1
3	C	2	ALA	2.1

### 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.