



# Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2020 – 03:40 pm BST

PDB ID : 5TJE  
Title : Murine class I major histocompatibility complex H-2Db in complex with LCMV-derived gp33 and T cell receptor P14  
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Deposited on : 2016-10-04  
Resolution : 3.20 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

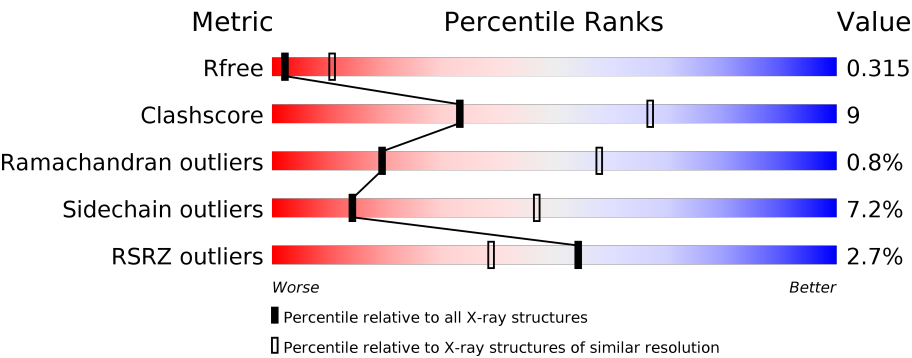
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.20 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	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	276	<div><div>%</div><div><div></div><div>77%</div><div>19%</div><div>.</div></div></div>
1	C	276	<div><div>3%</div><div><div></div><div>78%</div><div>19%</div><div>..</div></div></div>
2	B	99	<div><div></div><div><div></div><div>76%</div><div>22%</div><div>..</div></div></div>
2	D	99	<div><div>%</div><div><div></div><div>75%</div><div>22%</div><div>..</div></div></div>
3	E	205	<div><div></div><div><div></div><div>43%</div><div>11%</div><div>.</div><div>43%</div></div></div>
3	G	205	<div><div></div><div><div></div><div>45%</div><div>7%</div><div>.</div><div>45%</div></div></div>

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Mol	Chain	Length	Quality of chain
4	F	238	<div><div></div><div>3%</div><div>77%</div><div>21%</div><div></div></div>
4	H	238	<div><div></div><div>8%</div><div>74%</div><div>20%</div><div></div></div>
5	I	9	<div><div></div><div>33%</div><div>56%</div><div>11%</div><div></div></div>
5	J	9	<div><div></div><div>44%</div><div>33%</div><div>22%</div><div></div></div>

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 11784 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, D-B alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	275	Total	C	N	O	S	1	0	0
			2256	1425	398	424	9			
1	C	274	Total	C	N	O	S	1	0	0
			2248	1420	396	423	9			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	98	Total	C	N	O	S	0	0	0
			813	518	137	151	7			
2	D	98	Total	C	N	O	S	0	0	0
			813	518	137	151	7			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	85	ASP	ALA	conflict	UNP P01887
D	85	ASP	ALA	conflict	UNP P01887

- Molecule 3 is a protein called ALPHA CHAIN OF MURINE T CELL RECEPTOR p14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	112	Total	C	N	O	S	0	0	0
			880	567	140	171	2			
3	E	116	Total	C	N	O	S	0	0	0
			903	581	147	173	2			

- Molecule 4 is a protein called BETA CHAIN OF MURINE T CELL RECEPTOR p14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	232	Total	C	N	O	S	0	0	0
			1826	1146	326	348	6			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	237	Total	C	N	O	S	0	0	0
			1872	1176	333	357	6			

- Molecule 5 is a protein called Peptide gp33-41 from LCMV.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	I	9	Total	C	N	O	S	0	0	0
			73	48	11	13	1			
5	J	9	Total	C	N	O	S	0	0	0
			73	48	11	13	1			

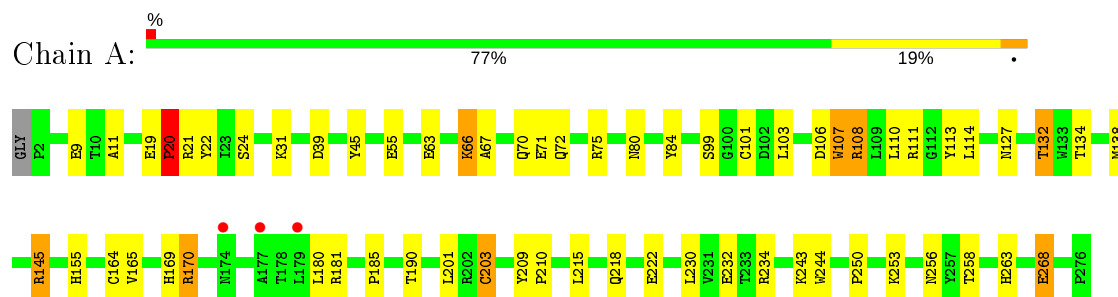
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	9	Total	O	0	0
			9	9		
6	B	4	Total	O	0	0
			4	4		
6	C	8	Total	O	0	0
			8	8		
6	H	2	Total	O	0	0
			2	2		
6	F	4	Total	O	0	0
			4	4		

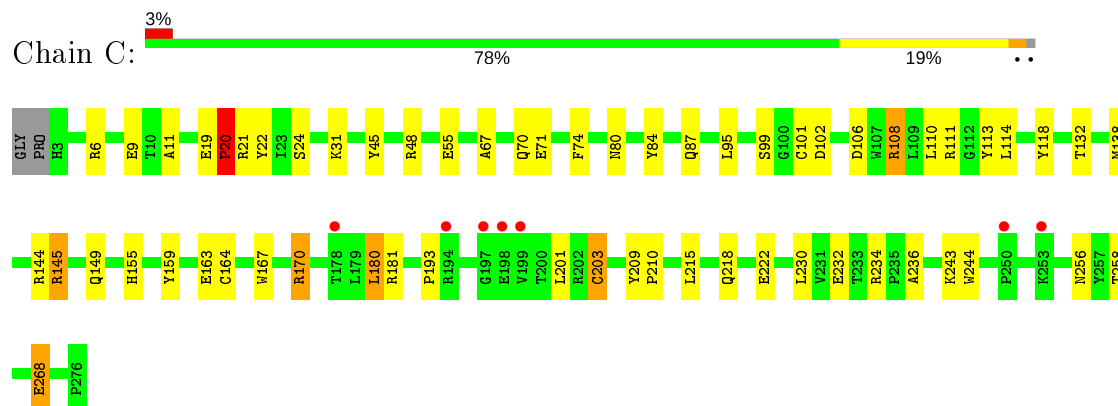
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

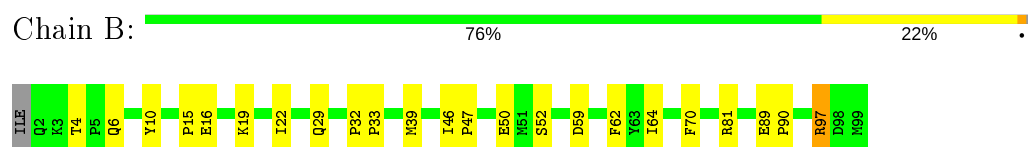
- Molecule 1: H-2 class I histocompatibility antigen, D-B alpha chain



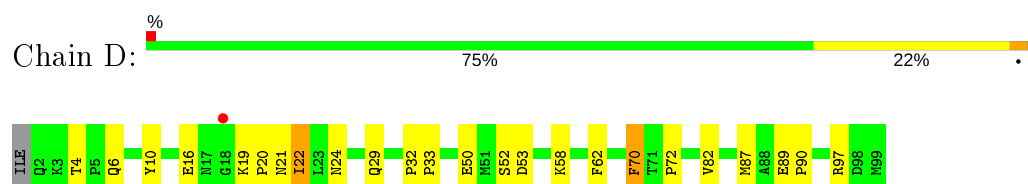
- Molecule 1: H-2 class I histocompatibility antigen, D-B alpha chain



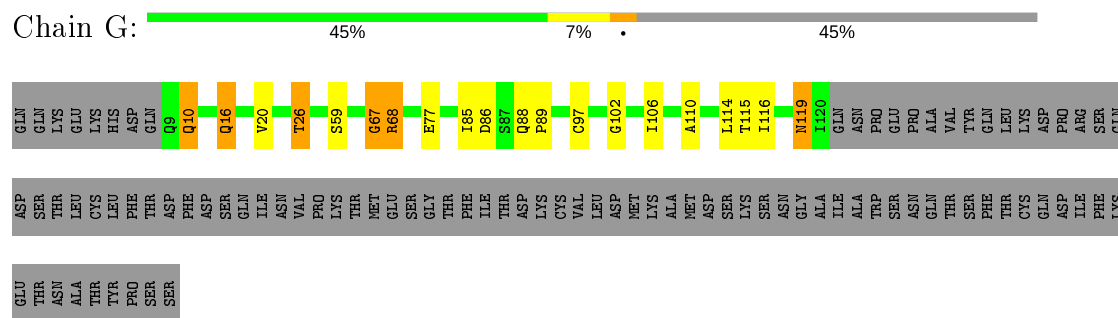
- Molecule 2: Beta-2-microglobulin



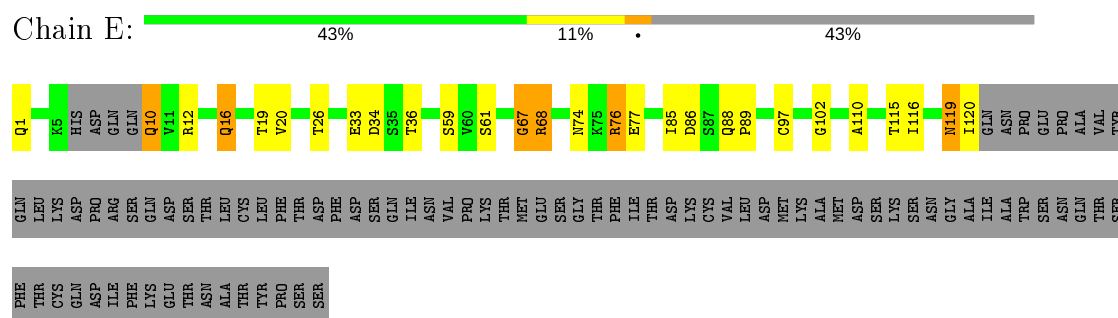
- Molecule 2: Beta-2-microglobulin



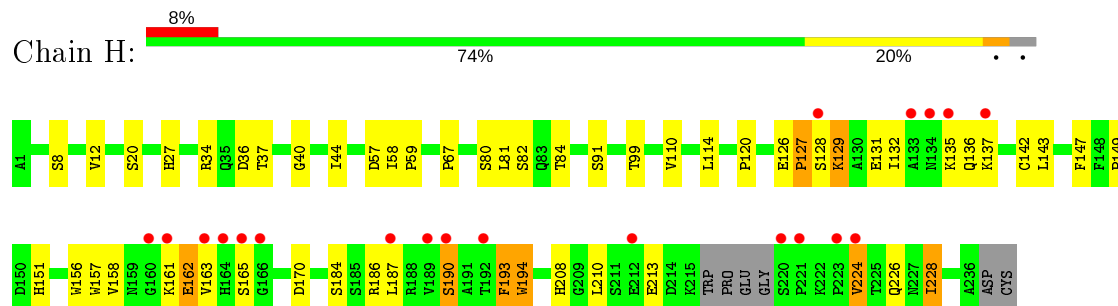
- Molecule 3: ALPHA CHAIN OF MURINE T CELL RECEPTOR p14



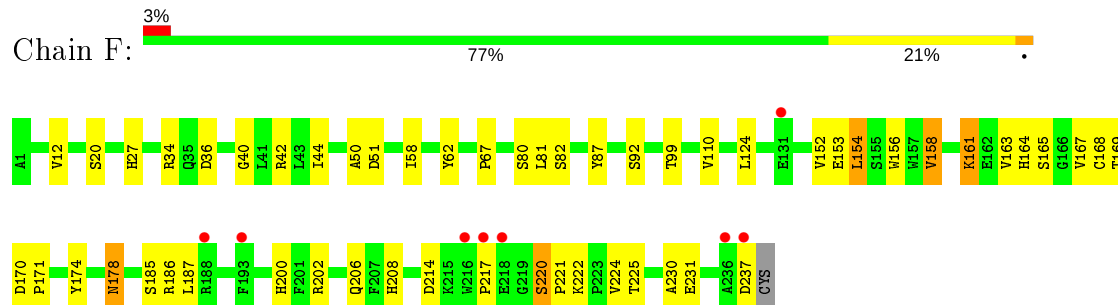
- Molecule 3: ALPHA CHAIN OF MURINE T CELL RECEPTOR p14



- Molecule 4: BETA CHAIN OF MURINE T CELL RECEPTOR p14

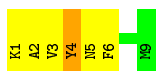


- Molecule 4: BETA CHAIN OF MURINE T CELL RECEPTOR p14

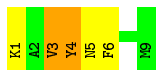


- Molecule 5: Peptide gp33-41 from LCMV





- Molecule 5: Peptide gp33-41 from LCMV





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	61.17Å 66.94Å 525.39Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.88 – 3.20 38.88 – 3.20	Depositor EDS
% Data completeness (in resolution range)	94.7 (38.88-3.20) 94.8 (38.88-3.20)	Depositor EDS
$R_{merge}$	0.17	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.73 (at 3.18Å)	Xtriage
Refinement program	REFMAC 5.8.0124	Depositor
R, $R_{free}$	0.228 , 0.314 0.234 , 0.315	Depositor DCC
$R_{free}$ test set	1825 reflections (5.20%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	77.2	Xtriage
Anisotropy	0.160	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 75.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.36$ , $\langle L^2 \rangle = 0.18$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	11784	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.22% 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 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	0.73	1/2323 (0.0%)	0.89	2/3156 (0.1%)
1	C	0.70	1/2313 (0.0%)	0.88	4/3141 (0.1%)
2	B	0.73	0/839	0.95	2/1137 (0.2%)
2	D	0.72	0/839	0.94	2/1137 (0.2%)
3	E	0.72	0/925	0.91	2/1254 (0.2%)
3	G	0.73	0/903	0.94	2/1226 (0.2%)
4	F	0.71	0/1924	0.86	2/2615 (0.1%)
4	H	0.68	0/1873	0.90	5/2542 (0.2%)
5	I	0.84	0/74	1.08	0/97
5	J	0.82	0/74	1.08	1/97 (1.0%)
All	All	0.71	2/12087 (0.0%)	0.90	22/16402 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
4	H	0	2
All	All	0	3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	20	PRO	N-CD	5.17	1.55	1.47
1	A	20	PRO	N-CD	5.15	1.55	1.47

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	194	TRP	CB-CA-C	-9.30	91.79	110.40
2	D	97	ARG	NE-CZ-NH1	9.12	124.86	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	97	ARG	NE-CZ-NH1	8.05	124.33	120.30
3	G	68	ARG	CB-CA-C	-7.54	95.32	110.40
4	H	128	SER	CB-CA-C	7.28	123.93	110.10
3	E	68	ARG	CB-CA-C	-6.87	96.67	110.40
4	F	202	ARG	NE-CZ-NH2	-6.40	117.10	120.30
4	F	202	ARG	NE-CZ-NH1	6.14	123.37	120.30
1	C	144	ARG	NE-CZ-NH1	6.05	123.33	120.30
1	A	268	GLU	OE1-CD-OE2	-5.83	116.30	123.30
4	H	190	SER	CB-CA-C	-5.48	99.69	110.10
4	H	193	PHE	N-CA-C	-5.47	96.22	111.00
3	G	67	GLY	N-CA-C	5.45	126.72	113.10
1	A	19	GLU	C-N-CD	5.43	139.79	128.40
4	H	129	LYS	CB-CA-C	-5.41	99.58	110.40
2	D	97	ARG	NE-CZ-NH2	-5.37	117.61	120.30
1	C	19	GLU	C-N-CD	5.36	139.66	128.40
2	B	97	ARG	NE-CZ-NH2	-5.30	117.65	120.30
5	J	3	VAL	CB-CA-C	-5.25	101.43	111.40
1	C	268	GLU	OE1-CD-OE2	-5.24	117.01	123.30
1	C	180	LEU	CA-CB-CG	5.02	126.85	115.30
3	E	67	GLY	N-CA-C	5.01	125.62	113.10

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	107	TRP	Peptide
4	H	129	LYS	Peptide
4	H	135	LYS	Peptide

## 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	2256	0	2120	40	1
1	C	2248	0	2118	31	0
2	B	813	0	782	16	0
2	D	813	0	782	16	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	903	0	864	16	0
3	G	880	0	845	12	0
4	F	1872	0	1784	32	0
4	H	1826	0	1741	41	0
5	I	73	0	74	15	0
5	J	73	0	74	8	0
6	A	9	0	0	0	0
6	B	4	0	0	0	0
6	C	8	0	0	2	0
6	F	4	0	0	1	0
6	H	2	0	0	0	0
All	All	11784	0	11184	197	1

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 9.

All (197) 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)
4:H:157:TRP:CE3	4:H:162:GLU:HB2	1.56	1.41
4:H:194:TRP:CG	4:H:194:TRP:O	2.08	1.05
4:F:158:VAL:O	4:F:200:HIS:O	1.76	1.00
4:H:157:TRP:CZ3	4:H:162:GLU:HB2	1.99	0.96
2:B:15:PRO:HG2	2:B:97:ARG:CG	2.01	0.91
4:H:157:TRP:CE3	4:H:162:GLU:CB	2.52	0.91
2:B:15:PRO:CG	2:B:97:ARG:HG3	2.01	0.90
4:H:157:TRP:HE3	4:H:162:GLU:HB2	1.28	0.87
1:A:66:LYS:CE	5:I:2:ALA:O	2.22	0.87
2:B:15:PRO:HG2	2:B:97:ARG:HG3	1.57	0.86
1:A:63:GLU:OE2	1:A:66:LYS:NZ	2.11	0.83
1:C:159:TYR:OH	5:J:1:LYS:O	1.98	0.82
1:A:11:ALA:HA	1:A:21:ARG:O	1.80	0.81
4:H:157:TRP:CZ3	4:H:162:GLU:CB	2.65	0.79
2:D:33:PRO:HB3	2:D:62:PHE:CE2	2.19	0.78
4:H:194:TRP:CD2	4:H:194:TRP:O	2.37	0.77
1:C:145:ARG:HG3	6:C:307:HOH:O	1.84	0.76
1:C:209:TYR:CD1	1:C:210:PRO:HA	2.22	0.75
4:H:190:SER:O	4:H:193:PHE:O	2.05	0.74
1:C:99:SER:HB3	5:J:3:VAL:HG21	1.70	0.73
2:B:15:PRO:HG3	2:B:97:ARG:HG3	1.71	0.71
1:A:66:LYS:HZ3	5:I:2:ALA:HB3	1.55	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:66:LYS:HE3	5:I:2:ALA:O	1.90	0.71
4:H:194:TRP:CD1	4:H:194:TRP:O	2.45	0.69
1:A:99:SER:HB3	5:I:3:VAL:HG21	1.75	0.69
1:A:209:TYR:CD1	1:A:210:PRO:HA	2.28	0.68
2:B:33:PRO:HB3	2:B:62:PHE:CE2	2.27	0.68
1:A:66:LYS:HE2	5:I:2:ALA:O	1.96	0.66
3:G:20:VAL:HG23	3:G:116:ILE:HD13	1.77	0.66
3:E:20:VAL:HG23	3:E:116:ILE:HD13	1.79	0.65
1:A:66:LYS:HD2	5:I:4:TYR:HD2	1.62	0.65
3:G:102:GLY:HA2	5:I:4:TYR:CE2	2.34	0.63
2:D:4:THR:O	2:D:6:GLN:NE2	2.31	0.63
1:A:66:LYS:NZ	5:I:2:ALA:HB3	2.13	0.63
1:A:63:GLU:CD	5:I:1:LYS:HG2	2.20	0.62
4:F:222:LYS:HB3	4:F:224:VAL:HG13	1.81	0.62
3:E:88:GLN:C	3:E:116:ILE:HG21	2.21	0.61
1:A:107:TRP:HB3	1:A:169:HIS:CE1	2.35	0.61
1:A:107:TRP:HB3	1:A:169:HIS:NE2	2.17	0.60
4:H:126:GLU:HB3	4:H:127:PRO:HD2	1.84	0.58
1:C:45:TYR:HE2	1:C:67:ALA:HB2	1.68	0.58
4:H:80:SER:O	4:H:110:VAL:HG11	2.03	0.58
3:G:88:GLN:C	3:G:116:ILE:HG21	2.24	0.57
1:C:11:ALA:HA	1:C:21:ARG:O	2.04	0.57
4:H:163:VAL:O	4:H:163:VAL:HG13	2.04	0.57
3:E:89:PRO:HA	3:E:116:ILE:HB	1.87	0.57
1:A:180:LEU:HD12	1:A:181:ARG:N	2.20	0.56
2:B:15:PRO:HG2	2:B:97:ARG:CD	2.36	0.56
3:E:1:GLN:HA	3:E:19:THR:O	2.06	0.56
1:C:180:LEU:HD12	1:C:181:ARG:N	2.20	0.55
2:B:15:PRO:HG2	2:B:97:ARG:HD2	1.89	0.55
4:H:8:SER:HB3	4:H:208:HIS:CD2	2.42	0.54
3:G:89:PRO:HA	3:G:116:ILE:HB	1.91	0.53
1:A:9:GLU:HG2	1:A:24:SER:OG	2.08	0.53
2:D:89:GLU:HB2	2:D:90:PRO:HD2	1.90	0.53
4:H:137:LYS:HG2	4:H:190:SER:HA	1.91	0.53
4:H:120:PRO:HG2	4:H:228:ILE:HD13	1.90	0.53
4:H:114:LEU:HD13	4:H:210:LEU:HG	1.91	0.53
3:E:10:GLN:HA	3:E:10:GLN:NE2	2.25	0.52
4:F:58:ILE:HG22	4:F:58:ILE:O	2.09	0.52
3:E:74:ASN:OD1	3:E:76:ARG:NH1	2.43	0.52
4:F:62:TYR:HH	4:F:87:TYR:HH	1.46	0.52
4:F:81:LEU:N	6:F:301:HOH:O	2.42	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:111:ARG:HD3	1:A:113:TYR:CE1	2.45	0.51
4:F:156:TRP:HZ2	4:F:185:SER:HG	1.59	0.51
2:B:32:PRO:CB	2:B:33:PRO:CD	2.88	0.51
3:G:119:ASN:OD1	3:G:119:ASN:C	2.48	0.51
2:B:89:GLU:HB2	2:B:90:PRO:HD2	1.92	0.51
3:E:16:GLN:N	3:E:16:GLN:OE1	2.43	0.51
2:B:16:GLU:O	2:B:19:LYS:HB2	2.11	0.51
4:F:158:VAL:HG23	4:F:163:VAL:HG21	1.93	0.51
4:F:158:VAL:HG23	4:F:163:VAL:CG2	2.41	0.51
3:G:16:GLN:OE1	3:G:16:GLN:N	2.44	0.50
1:A:63:GLU:HG2	5:I:1:LYS:HE2	1.93	0.50
3:E:102:GLY:HA2	5:J:4:TYR:CE2	2.46	0.50
3:E:67:GLY:O	3:E:68:ARG:HB2	2.12	0.50
4:F:169:THR:HA	4:F:185:SER:CB	2.42	0.50
3:E:68:ARG:HA	3:E:85:ILE:HD12	1.94	0.50
4:F:62:TYR:OH	4:F:87:TYR:OH	2.19	0.50
1:A:66:LYS:HD2	5:I:4:TYR:CD2	2.46	0.49
1:C:106:ASP:O	1:C:108:ARG:N	2.45	0.49
3:E:119:ASN:C	3:E:119:ASN:OD1	2.51	0.49
4:F:153:GLU:OE1	4:F:208:HIS:HE1	1.95	0.49
4:F:154:LEU:HD23	4:F:154:LEU:C	2.32	0.49
1:C:234:ARG:HD3	2:D:10:TYR:CZ	2.47	0.49
4:H:132:ILE:O	4:H:136:GLN:HG2	2.13	0.49
1:A:127:ASN:HD21	1:A:134:THR:HG1	1.60	0.49
1:C:167:TRP:CZ2	5:J:1:LYS:HD2	2.48	0.49
1:C:234:ARG:HD3	2:D:10:TYR:CE1	2.48	0.49
4:F:27:HIS:HB3	4:F:92:SER:O	2.12	0.49
1:A:70:GLN:HE22	5:I:5:ASN:HB2	1.79	0.48
4:H:142:CYS:HB2	4:H:156:TRP:CH2	2.49	0.48
4:F:124:LEU:HB3	4:F:230:ALA:HB1	1.95	0.48
1:A:31:LYS:HD3	1:A:209:TYR:OH	2.14	0.48
1:C:111:ARG:HD3	1:C:113:TYR:CE1	2.49	0.48
4:F:220:SER:CB	4:F:221:PRO:CD	2.92	0.48
4:F:220:SER:HB3	4:F:221:PRO:CD	2.43	0.48
1:A:66:LYS:HZ1	5:I:2:ALA:N	2.11	0.48
1:C:80:ASN:O	1:C:84:TYR:CD1	2.67	0.47
2:D:16:GLU:O	2:D:19:LYS:HB2	2.14	0.47
1:A:106:ASP:O	1:A:108:ARG:N	2.48	0.47
4:H:27:HIS:ND1	4:H:91:SER:OG	2.36	0.47
4:F:152:VAL:HA	4:F:206:GLN:O	2.14	0.47
2:D:32:PRO:CB	2:D:33:PRO:CD	2.91	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:143:LEU:HD12	4:H:184:SER:HB3	1.96	0.47
4:H:186:ARG:C	4:H:187:LEU:N	2.68	0.47
1:A:234:ARG:HD3	2:B:10:TYR:CZ	2.49	0.47
1:C:163:GLU:O	1:C:167:TRP:HD1	1.98	0.47
3:G:110:ALA:O	4:H:40:GLY:N	2.47	0.47
1:C:48:ARG:NH2	2:D:53:ASP:OD2	2.48	0.47
4:F:167:VAL:HG12	4:F:168:CYS:N	2.29	0.47
1:C:215:LEU:HD11	1:C:243:LYS:HG2	1.97	0.47
4:H:36:ASP:O	4:H:37:THR:OG1	2.32	0.47
4:F:50:ALA:HB1	4:F:51:ASP:OD1	2.14	0.46
4:H:57:ASP:C	4:H:59:PRO:HD3	2.35	0.46
1:A:55:GLU:OE1	1:A:170:ARG:NH1	2.49	0.46
4:H:58:ILE:O	4:H:58:ILE:HG22	2.15	0.46
4:F:156:TRP:CD1	4:F:156:TRP:N	2.83	0.46
3:E:110:ALA:O	4:F:40:GLY:N	2.48	0.46
1:C:203:CYS:O	1:C:244:TRP:HA	2.16	0.46
4:H:131:GLU:O	4:H:136:GLN:N	2.48	0.46
4:H:151:HIS:HB3	4:H:208:HIS:HB2	1.98	0.46
1:A:185:PRO:HD3	1:A:263:HIS:CD2	2.51	0.46
1:C:55:GLU:OE1	1:C:170:ARG:NH1	2.48	0.46
1:C:70:GLN:HE22	5:J:5:ASN:HB2	1.81	0.46
4:H:157:TRP:CZ3	4:H:162:GLU:HB3	2.47	0.46
1:A:72:GLN:OE1	1:A:75:ARG:NH1	2.49	0.45
1:C:155:HIS:HB3	5:J:6:PHE:CZ	2.51	0.45
1:A:21:ARG:HH21	1:A:39:ASP:HB2	1.81	0.45
1:A:22:TYR:HB3	1:A:71:GLU:HG3	1.97	0.45
1:C:45:TYR:CE2	1:C:67:ALA:HB2	2.49	0.45
1:A:218:GLN:HA	1:A:222:GLU:O	2.17	0.45
4:H:114:LEU:HD13	4:H:210:LEU:CG	2.46	0.45
2:D:21:ASN:OD1	2:D:22:ILE:N	2.44	0.45
1:A:190:THR:O	1:A:201:LEU:HA	2.16	0.44
1:A:80:ASN:O	1:A:84:TYR:CD1	2.69	0.44
1:C:87:GLN:NE2	1:C:118:TYR:OH	2.49	0.44
1:A:103:LEU:HD11	1:A:165:VAL:HG22	1.98	0.44
3:E:10:GLN:HE21	3:E:10:GLN:HA	1.83	0.44
4:H:156:TRP:CE3	4:H:187:LEU:HD23	2.52	0.44
3:G:10:GLN:NE2	3:G:10:GLN:HA	2.32	0.44
3:G:26:THR:HG21	3:G:114:LEU:HD11	1.98	0.44
2:D:33:PRO:HB3	2:D:62:PHE:CD2	2.53	0.44
4:H:84:THR:HG23	4:H:84:THR:O	2.18	0.44
1:A:203:CYS:O	1:A:244:TRP:HA	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:67:GLY:O	3:G:68:ARG:HB2	2.18	0.43
1:A:45:TYR:HE2	1:A:67:ALA:HB2	1.82	0.43
4:F:80:SER:O	4:F:110:VAL:HG11	2.18	0.43
1:A:215:LEU:HD11	1:A:243:LYS:HG2	1.99	0.43
1:C:22:TYR:HB3	1:C:71:GLU:HG3	2.01	0.43
4:F:169:THR:HA	4:F:185:SER:HB3	1.99	0.43
3:G:106:ILE:O	3:G:106:ILE:HG23	2.19	0.43
2:B:52:SER:HB3	2:B:64:ILE:HG13	2.01	0.43
3:E:34:ASP:OD1	3:E:36:THR:OG1	2.26	0.43
2:B:32:PRO:CB	2:B:33:PRO:HD2	2.48	0.42
2:D:19:LYS:O	2:D:72:PRO:HD2	2.19	0.42
2:D:32:PRO:CB	2:D:33:PRO:HD2	2.49	0.42
4:F:158:VAL:CG2	4:F:163:VAL:HG11	2.49	0.42
4:F:178:ASN:N	4:F:178:ASN:OD1	2.50	0.42
1:C:218:GLN:HA	1:C:222:GLU:O	2.20	0.42
1:C:9:GLU:HG2	1:C:24:SER:OG	2.20	0.42
4:F:36:ASP:OD2	4:F:42:ARG:NH1	2.52	0.42
4:F:34:ARG:HB2	4:F:44:ILE:HD11	2.00	0.42
3:G:68:ARG:HA	3:G:85:ILE:HD12	2.02	0.42
2:B:4:THR:O	2:B:6:GLN:NE2	2.53	0.42
1:A:155:HIS:HB3	5:I:6:PHE:CE2	2.55	0.42
3:E:12:ARG:NH2	3:E:33:GLU:OE1	2.53	0.42
4:F:152:VAL:HG23	4:F:152:VAL:O	2.20	0.42
4:H:149:PRO:O	4:H:151:HIS:N	2.53	0.42
2:B:59:ASP:N	2:B:59:ASP:OD1	2.53	0.42
2:D:82:VAL:HG12	2:D:87:MET:HE1	2.02	0.42
4:H:224:VAL:HG23	4:H:226:GLN:NE2	2.35	0.42
1:A:155:HIS:CB	5:I:6:PHE:CE2	3.03	0.42
1:A:127:ASN:HB2	1:A:132:THR:HG22	2.02	0.42
4:H:80:SER:C	4:H:110:VAL:HG11	2.40	0.42
4:F:158:VAL:CG2	4:F:163:VAL:HG21	2.49	0.42
2:D:21:ASN:HB3	2:D:70:PHE:CE1	2.55	0.41
4:H:156:TRP:CD2	4:H:187:LEU:HD23	2.54	0.41
2:B:39:MET:O	2:B:46:ILE:HG13	2.20	0.41
1:C:236:ALA:O	2:D:24:ASN:ND2	2.52	0.41
4:H:34:ARG:HB2	4:H:44:ILE:HD11	2.01	0.41
1:C:31:LYS:HD3	1:C:209:TYR:OH	2.21	0.41
1:C:6:ARG:NH1	1:C:102:ASP:OD1	2.53	0.41
4:H:57:ASP:O	4:H:59:PRO:HD3	2.20	0.41
1:C:74:PHE:CD2	1:C:95:LEU:HD23	2.56	0.41
6:C:302:HOH:O	2:D:58:LYS:HE2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:190:SER:HB3	4:H:193:PHE:HB2	2.03	0.41
1:A:250:PRO:HG2	1:A:253:LYS:HG3	2.03	0.40
4:H:158:VAL:HG23	4:H:161:LYS:O	2.22	0.40
1:C:155:HIS:CB	5:J:6:PHE:CE2	3.05	0.40
3:E:119:ASN:O	3:E:120:ILE:HB	2.22	0.40
4:F:220:SER:HB3	4:F:221:PRO:HD3	2.04	0.40
4:H:120:PRO:HB3	4:H:147:PHE:HB3	2.03	0.40
4:H:81:LEU:O	4:H:84:THR:HG22	2.22	0.40
1:C:167:TRP:CE2	5:J:1:LYS:HD2	2.57	0.40
4:F:161:LYS:HD3	4:F:161:LYS:HA	1.65	0.40
4:F:170:ASP:HB3	4:F:171:PRO:CD	2.52	0.40

All (1) 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)
1:A:145:ARG:NH2	2:D:20:PRO:O[1_565]	2.05	0.15

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	273/276 (99%)	253 (93%)	19 (7%)	1 (0%)	34	69
1	C	272/276 (99%)	253 (93%)	17 (6%)	2 (1%)	22	61
2	B	96/99 (97%)	86 (90%)	9 (9%)	1 (1%)	15	54
2	D	96/99 (97%)	88 (92%)	8 (8%)	0	100	100
3	E	112/205 (55%)	101 (90%)	11 (10%)	0	100	100
3	G	110/205 (54%)	98 (89%)	12 (11%)	0	100	100
4	F	235/238 (99%)	211 (90%)	20 (8%)	4 (2%)	9	42

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	H	226/238 (95%)	197 (87%)	25 (11%)	4 (2%)	8	41
5	I	7/9 (78%)	5 (71%)	2 (29%)	0	100	100
5	J	7/9 (78%)	5 (71%)	2 (29%)	0	100	100
All	All	1434/1654 (87%)	1297 (90%)	125 (9%)	12 (1%)	19	58

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	F	217	PRO
1	A	20	PRO
4	H	67	PRO
4	F	67	PRO
4	F	220	SER
4	H	213	GLU
4	H	127	PRO
1	C	20	PRO
4	H	224	VAL
4	F	158	VAL
1	C	193	PRO
2	B	47	PRO

### 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	233/234 (100%)	216 (93%)	17 (7%)	14	46
1	C	232/234 (99%)	214 (92%)	18 (8%)	12	43
2	B	93/94 (99%)	88 (95%)	5 (5%)	22	58
2	D	93/94 (99%)	88 (95%)	5 (5%)	22	58
3	E	96/184 (52%)	85 (88%)	11 (12%)	5	24
3	G	96/184 (52%)	87 (91%)	9 (9%)	8	33
4	F	203/204 (100%)	187 (92%)	16 (8%)	12	43

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	H	198/204 (97%)	190 (96%)	8 (4%)	31	66
5	I	7/7 (100%)	6 (86%)	1 (14%)	3	15
5	J	7/7 (100%)	6 (86%)	1 (14%)	3	15
All	All	1258/1446 (87%)	1167 (93%)	91 (7%)	14	47

All (91) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	PRO
1	A	66	LYS
1	A	101	CYS
1	A	108	ARG
1	A	110	LEU
1	A	114	LEU
1	A	132	THR
1	A	138	MET
1	A	145	ARG
1	A	164	CYS
1	A	170	ARG
1	A	203	CYS
1	A	230	LEU
1	A	232	GLU
1	A	256	ASN
1	A	258	THR
1	A	268	GLU
2	B	22	ILE
2	B	29	GLN
2	B	50	GLU
2	B	70	PHE
2	B	81	ARG
1	C	20	PRO
1	C	101	CYS
1	C	108	ARG
1	C	110	LEU
1	C	114	LEU
1	C	132	THR
1	C	138	MET
1	C	145	ARG
1	C	149	GLN
1	C	164	CYS
1	C	170	ARG

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Mol	Chain	Res	Type
1	C	201	LEU
1	C	203	CYS
1	C	230	LEU
1	C	232	GLU
1	C	256	ASN
1	C	258	THR
1	C	268	GLU
2	D	22	ILE
2	D	29	GLN
2	D	50	GLU
2	D	52	SER
2	D	70	PHE
3	G	10	GLN
3	G	16	GLN
3	G	26	THR
3	G	59	SER
3	G	77	GLU
3	G	86	ASP
3	G	97	CYS
3	G	115	THR
3	G	119	ASN
4	H	12	VAL
4	H	20	SER
4	H	82	SER
4	H	99	THR
4	H	162	GLU
4	H	165	SER
4	H	170	ASP
4	H	228	ILE
3	E	10	GLN
3	E	16	GLN
3	E	26	THR
3	E	59	SER
3	E	61	SER
3	E	76	ARG
3	E	77	GLU
3	E	86	ASP
3	E	97	CYS
3	E	115	THR
3	E	119	ASN
4	F	12	VAL
4	F	20	SER

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Mol	Chain	Res	Type
4	F	82	SER
4	F	99	THR
4	F	154	LEU
4	F	161	LYS
4	F	164	HIS
4	F	165	SER
4	F	174	TYR
4	F	178	ASN
4	F	186	ARG
4	F	187	LEU
4	F	214	ASP
4	F	225	THR
4	F	231	GLU
4	F	237	ASP
5	I	4	TYR
5	J	4	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	70	GLN
1	A	87	GLN
1	A	127	ASN
1	A	220	ASN
1	A	263	HIS
2	B	8	GLN
2	B	13	HIS
1	C	70	GLN
1	C	87	GLN
1	C	220	ASN
2	D	2	GLN
2	D	8	GLN
2	D	13	HIS
3	G	10	GLN
3	G	44	GLN
4	H	69	GLN
4	H	199	ASN
4	H	208	HIS
4	H	226	GLN
3	E	10	GLN
4	F	69	GLN
4	F	172	GLN

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Mol	Chain	Res	Type
4	F	208	HIS
5	I	5	ASN
5	J	5	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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
4	H	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	H	186:ARG	C	187:LEU	N	2.68

## 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	275/276 (99%)	-0.14	3 (1%) 80 69	36, 72, 119, 153	1 (0%)
1	C	274/276 (99%)	-0.03	7 (2%) 56 40	39, 76, 115, 195	1 (0%)
2	B	98/99 (98%)	-0.27	0 100 100	41, 64, 90, 113	0
2	D	98/99 (98%)	-0.24	1 (1%) 82 72	43, 71, 104, 128	0
3	E	116/205 (56%)	-0.12	0 100 100	50, 74, 106, 129	0
3	G	112/205 (54%)	-0.16	0 100 100	41, 71, 102, 117	0
4	F	237/238 (99%)	0.09	8 (3%) 45 29	49, 83, 117, 142	0
4	H	232/238 (97%)	0.27	20 (8%) 10 5	44, 85, 141, 188	0
5	I	9/9 (100%)	-0.12	0 100 100	48, 52, 66, 72	0
5	J	9/9 (100%)	-0.06	0 100 100	39, 51, 67, 69	0
All	All	1460/1654 (88%)	-0.03	39 (2%) 54 39	36, 75, 119, 195	2 (0%)

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	H	163	VAL	5.6
1	C	178	THR	5.1
4	H	134	ASN	4.6
4	H	220	SER	4.2
1	A	177	ALA	4.1
4	F	236	ALA	3.9
4	H	164	HIS	3.4
4	F	237	ASP	3.4
4	H	187	LEU	3.3
4	H	212	GLU	3.2
1	C	253	LYS	3.1
1	C	197	GLY	3.1
4	H	133	ALA	3.1

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Mol	Chain	Res	Type	RSRZ
4	F	217	PRO	3.0
4	F	218	GLU	2.7
4	H	161	LYS	2.7
4	H	165	SER	2.7
4	H	192	THR	2.6
4	H	223	PRO	2.6
4	F	216	TRP	2.5
1	A	174	ASN	2.5
1	C	199	VAL	2.5
1	C	198	GLU	2.5
4	H	224	VAL	2.5
4	H	166	GLY	2.4
4	H	137	LYS	2.4
1	A	179	LEU	2.3
1	C	250	PRO	2.3
4	H	128	SER	2.3
4	H	189	VAL	2.3
4	H	135	LYS	2.3
4	H	160	GLY	2.2
4	H	190	SER	2.2
4	F	193	PHE	2.1
4	F	188	ARG	2.1
4	H	221	PRO	2.1
4	F	131	GLU	2.1
1	C	194	ARG	2.0
2	D	18	GLY	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.