



# Full wwPDB X-ray Structure Validation Report ⓘ

Jul 7, 2021 – 12:06 PM EDT

PDB ID : 7MFA  
Title : Crystal structure of antibody 10E8v4-P100fA+P100gA Fab  
Authors : Kwon, Y.D.; Kwong, P.D.  
Deposited on : 2021-04-08  
Resolution : 2.40 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	:	2.22
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)	:	2.22

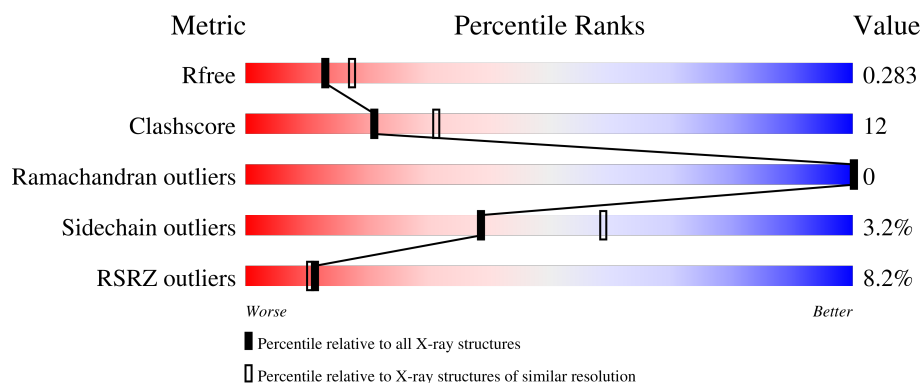
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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	C	233	<div> <div>3%</div> <div>76%</div> <div>20%</div> <div>..</div> </div>
1	G	233	<div> <div>9%</div> <div>67%</div> <div>27%</div> <div>..</div> </div>
1	H	233	<div> <div>7%</div> <div>69%</div> <div>27%</div> <div>.</div> </div>
1	M	233	<div> <div>10%</div> <div>66%</div> <div>30%</div> <div>.</div> </div>
1	Q	233	<div> <div>8%</div> <div>61%</div> <div>34%</div> <div>..</div> </div>

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
1	U	233	
2	D	215	
2	I	215	
2	L	215	
2	N	215	
2	R	215	
2	V	215	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 19719 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 Antibody 10E8v4 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	224	Total	C	N	O	S	0	0	0
			1708	1085	284	333	6			
1	C	225	Total	C	N	O	S	0	0	0
			1720	1094	286	334	6			
1	G	224	Total	C	N	O	S	0	0	0
			1711	1088	285	332	6			
1	M	224	Total	C	N	O	S	0	0	0
			1697	1077	284	330	6			
1	Q	223	Total	C	N	O	S	0	0	0
			1707	1087	284	330	6			
1	U	224	Total	C	N	O	S	0	0	0
			1699	1076	285	332	6			

- Molecule 2 is a protein called Antibody 10E8v4 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	209	Total	C	N	O	S	0	0	0
			1569	978	271	316	4			
2	D	209	Total	C	N	O	S	0	0	0
			1569	978	271	316	4			
2	I	210	Total	C	N	O	S	0	0	0
			1575	981	272	318	4			
2	N	209	Total	C	N	O	S	0	0	0
			1573	981	272	316	4			
2	R	209	Total	C	N	O	S	0	0	0
			1550	963	269	314	4			
2	V	209	Total	C	N	O	S	0	0	0
			1559	967	272	316	4			

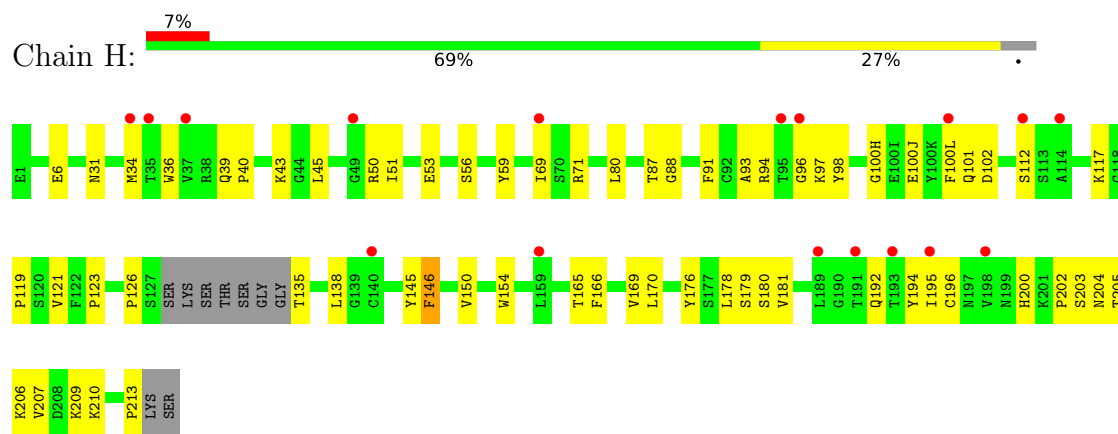
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	H	9	Total 9	O 9	0	0
3	L	14	Total 14	O 14	0	0
3	C	17	Total 17	O 17	0	0
3	D	10	Total 10	O 10	0	0
3	G	7	Total 7	O 7	0	0
3	I	6	Total 6	O 6	0	0
3	M	4	Total 4	O 4	0	0
3	N	10	Total 10	O 10	0	0
3	Q	3	Total 3	O 3	0	0
3	U	1	Total 1	O 1	0	0
3	V	1	Total 1	O 1	0	0

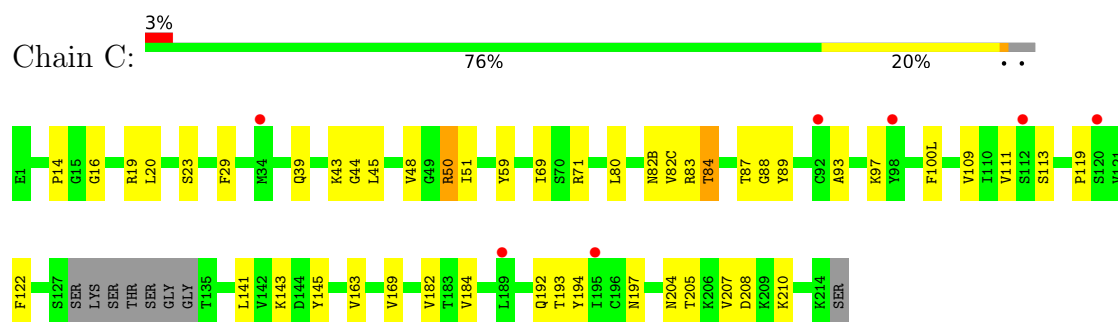
### 3 Residue-property plots [i](#)

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.

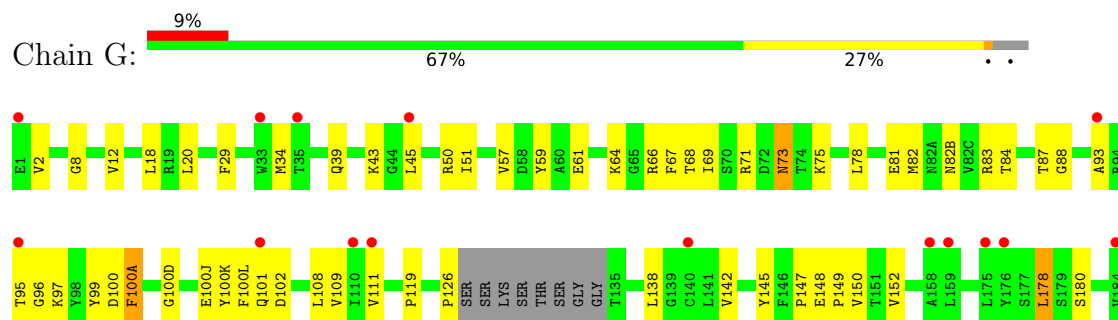
- Molecule 1: Antibody 10E8v4 Fab heavy chain

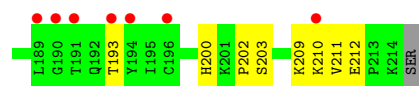


- Molecule 1: Antibody 10E8v4 Fab heavy chain

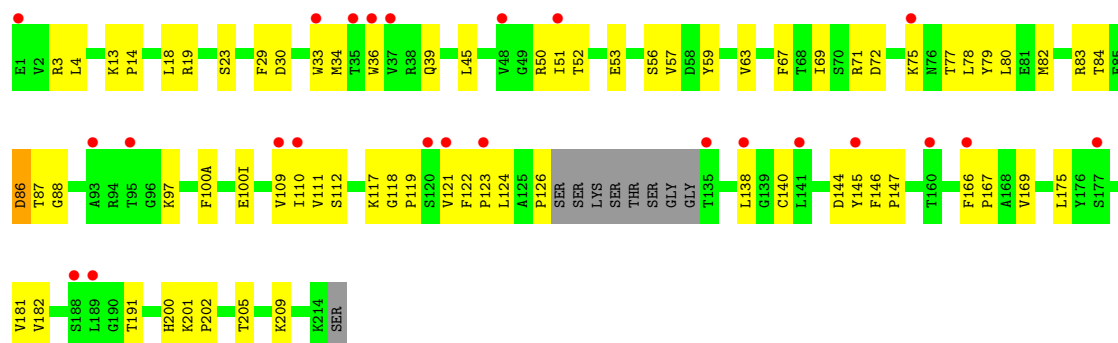


- Molecule 1: Antibody 10E8v4 Fab heavy chain

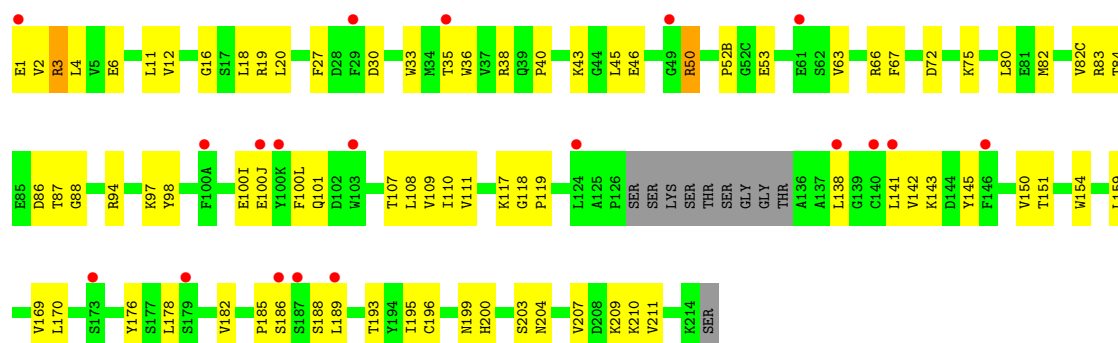




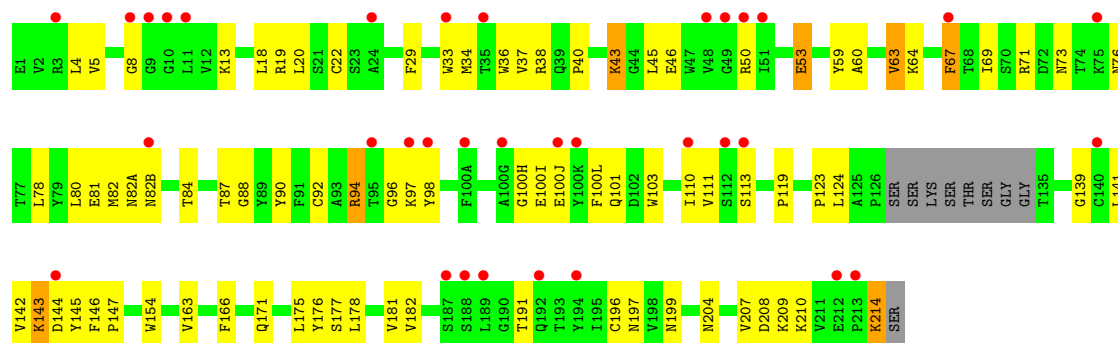
• Molecule 1: Antibody 10E8v4 Fab heavy chain



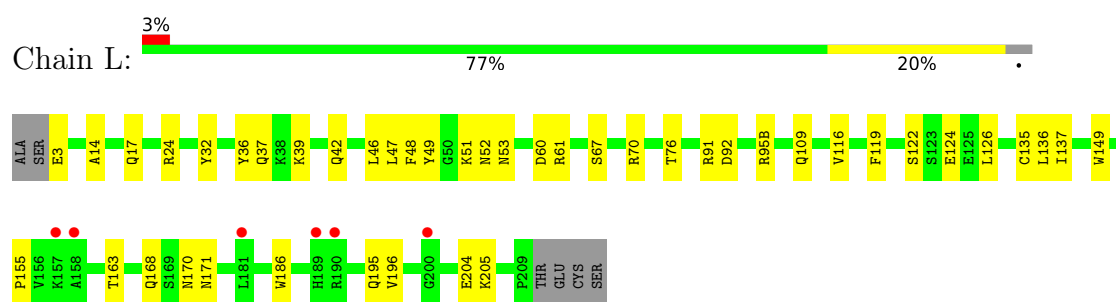
• Molecule 1: Antibody 10E8v4 Fab heavy chain



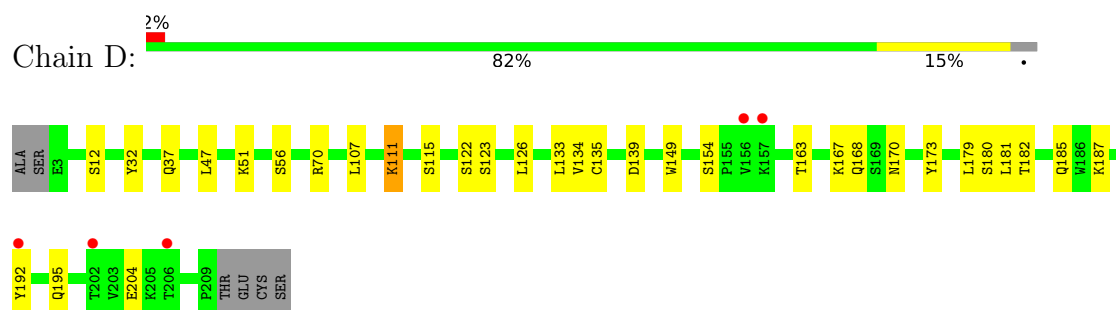
• Molecule 1: Antibody 10E8v4 Fab heavy chain



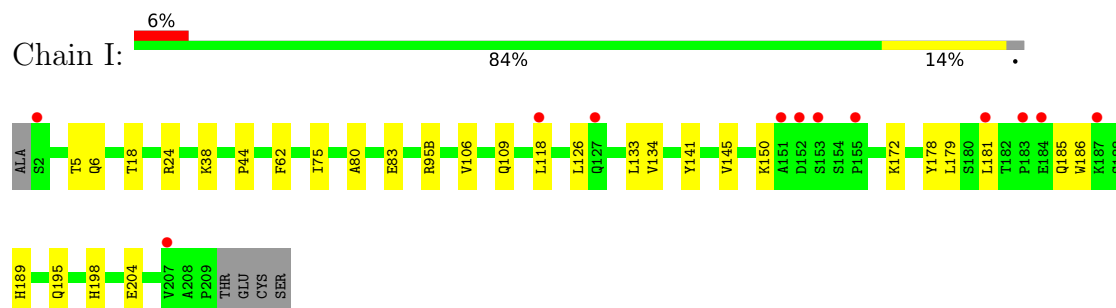
• Molecule 2: Antibody 10E8v4 Fab light chain



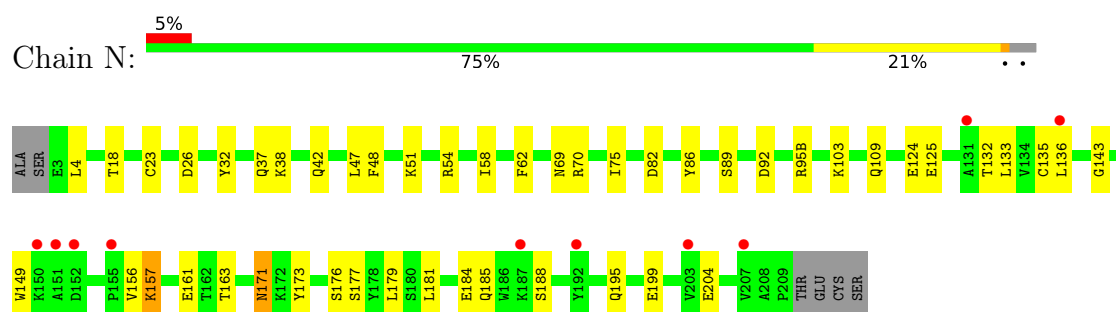
- Molecule 2: Antibody 10E8v4 Fab light chain



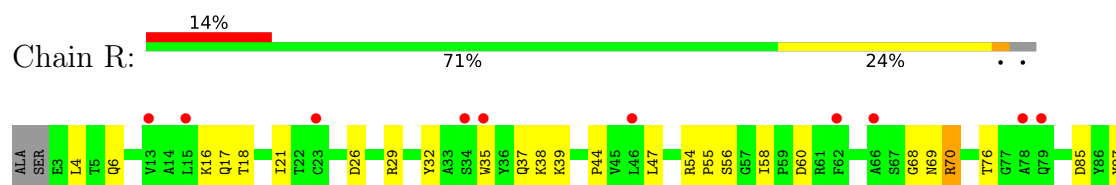
- Molecule 2: Antibody 10E8v4 Fab light chain



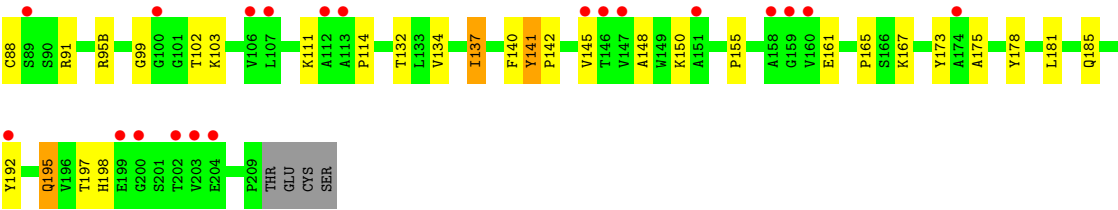
- Molecule 2: Antibody 10E8v4 Fab light chain



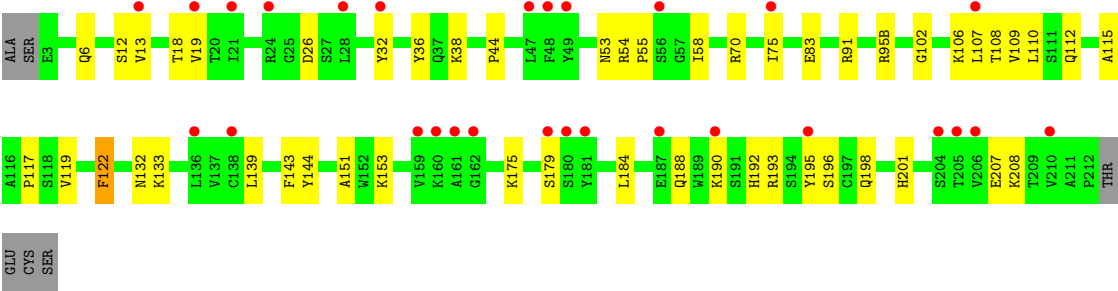
- Molecule 2: Antibody 10E8v4 Fab light chain







● Molecule 2: Antibody 10E8v4 Fab light chain



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	95.78Å 53.80Å 328.53Å 90.00° 90.60° 90.00°	Depositor
Resolution (Å)	35.01 – 2.40 35.01 – 2.39	Depositor EDS
% Data completeness (in resolution range)	78.3 (35.01-2.40) 78.4 (35.01-2.39)	Depositor EDS
$R_{merge}$	0.15	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.08 (at 2.39Å)	Xtriage
Refinement program	PHENIX 1.19.1_4122	Depositor
R, $R_{free}$	0.238 , 0.286 0.239 , 0.283	Depositor DCC
$R_{free}$ test set	1902 reflections (1.81%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	68.3	Xtriage
Anisotropy	0.369	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 56.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.022 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	19719	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	99.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.81% 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	C	0.28	0/1767	0.54	0/2406
1	G	0.31	0/1758	0.57	0/2394
1	H	0.29	0/1755	0.53	0/2391
1	M	0.30	0/1743	0.54	0/2374
1	Q	0.28	0/1754	0.54	0/2388
1	U	0.37	1/1744 (0.1%)	0.60	2/2376 (0.1%)
2	D	0.27	0/1605	0.54	0/2186
2	I	0.27	0/1611	0.52	0/2194
2	L	0.31	0/1605	0.55	0/2186
2	N	0.27	0/1609	0.53	0/2190
2	R	0.27	0/1586	0.54	0/2161
2	V	0.28	0/1593	0.55	0/2169
All	All	0.29	1/20130 (0.0%)	0.55	2/27415 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	U	67	PHE	CE1-CZ	7.73	1.52	1.37

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	U	143	LYS	CA-CB-CG	5.38	125.23	113.40
1	U	63	VAL	N-CA-CB	-5.20	100.06	111.50

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	C	1720	0	1655	35	0
1	G	1711	0	1641	49	0
1	H	1708	0	1633	49	0
1	M	1697	0	1619	51	0
1	Q	1707	0	1643	68	0
1	U	1699	0	1627	74	0
2	D	1569	0	1529	18	0
2	I	1575	0	1534	20	0
2	L	1569	0	1529	33	0
2	N	1573	0	1540	33	0
2	R	1550	0	1477	37	0
2	V	1559	0	1519	39	0
3	C	17	0	0	3	0
3	D	10	0	0	1	0
3	G	7	0	0	2	0
3	H	9	0	0	5	0
3	I	6	0	0	0	0
3	L	14	0	0	1	0
3	M	4	0	0	1	0
3	N	10	0	0	2	0
3	Q	3	0	0	0	0
3	U	1	0	0	0	0
3	V	1	0	0	0	0
All	All	19719	0	18946	465	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 12.

All (465) 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:M:169:VAL:HG11	2:N:161:GLU:HB3	1.39	1.03
2:V:112:GLN:HE22	2:V:175:LYS:HD3	1.32	0.94
1:U:97:LYS:HE2	1:U:100(J):GLU:HG2	1.50	0.92
1:M:100(I):GLU:OE1	3:M:301:HOH:O	1.87	0.91
1:M:77:THR:HG1	1:M:79:TYR:HE1	1.18	0.90
2:D:70:ARG:NH1	3:D:301:HOH:O	2.04	0.90
1:G:193:THR:HB	1:G:210:LYS:HZ1	1.37	0.89
1:Q:195:ILE:HD11	1:Q:210:LYS:HG2	1.54	0.89

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:135:THR:N	3:H:302:HOH:O	2.07	0.88
1:U:59:TYR:HE1	1:U:69:ILE:HG13	1.40	0.86
1:Q:141:LEU:HD21	1:Q:143:LYS:HG3	1.57	0.84
1:M:123:PRO:HD3	1:M:209:LYS:HD3	1.60	0.82
1:U:181:VAL:HG21	2:V:139:LEU:HD11	1.61	0.79
1:U:33:TRP:HE3	1:U:97:LYS:HZ2	1.30	0.79
1:Q:20:LEU:HD11	1:Q:107:THR:HG21	1.65	0.78
1:Q:169:VAL:HG21	2:R:161:GLU:HB3	1.66	0.78
1:H:50:ARG:NH2	3:H:301:HOH:O	2.02	0.77
1:U:197:ASN:ND2	1:U:208:ASP:OD2	2.17	0.77
1:Q:94:ARG:HD3	1:Q:101:GLN:HE21	1.49	0.76
1:H:195:ILE:HG12	1:H:210:LYS:HG2	1.66	0.76
2:L:3:GLU:N	3:L:301:HOH:O	2.19	0.76
2:R:141:TYR:HD1	2:R:142:PRO:HA	1.50	0.76
1:M:56:SER:OG	2:N:95(B):ARG:NH2	2.20	0.73
1:U:63:VAL:HG13	1:U:67:PHE:HD1	1.54	0.72
1:C:48:VAL:O	3:C:301:HOH:O	2.06	0.72
1:Q:117:LYS:NZ	1:Q:118:GLY:O	2.23	0.71
1:H:169:VAL:HB	2:L:163:THR:HG22	1.72	0.71
2:R:38:LYS:HD3	2:R:44:PRO:HG3	1.72	0.71
2:R:181:LEU:HD22	2:R:185:GLN:HB2	1.71	0.70
1:Q:40:PRO:HB2	1:Q:43:LYS:HD2	1.73	0.70
1:H:31:ASN:OD1	3:H:303:HOH:O	2.10	0.69
1:H:207:VAL:HG22	1:Q:207:VAL:HG22	1.75	0.69
2:D:167:LYS:NZ	2:D:173:TYR:OH	2.25	0.69
1:G:95:THR:HG22	1:G:100(L):PHE:HD1	1.57	0.69
1:M:51:ILE:HG13	1:M:57:VAL:HG22	1.73	0.69
2:N:69:ASN:OD1	2:N:70:ARG:NH1	2.25	0.69
1:U:100(L):PHE:N	2:V:36:TYR:OH	2.25	0.69
2:I:83:GLU:HB2	2:I:106:VAL:HG22	1.75	0.68
1:G:101:GLN:OE1	3:G:301:HOH:O	2.10	0.68
1:M:121:VAL:HG12	1:M:209:LYS:HD2	1.75	0.68
1:U:13:LYS:HG3	1:U:113:SER:HA	1.76	0.68
2:V:83:GLU:HG3	2:V:109:VAL:H	1.58	0.68
2:V:192:HIS:CE1	2:V:195:TYR:HH	2.10	0.68
1:M:126:PRO:HG3	1:M:138:LEU:HB3	1.76	0.68
1:M:167:PRO:HG2	2:N:163:THR:HB	1.76	0.67
2:R:141:TYR:CD1	2:R:142:PRO:HA	2.30	0.67
1:U:100(I):GLU:HA	2:V:91:ARG:HH21	1.60	0.67
1:H:93:ALA:HB1	1:H:100(L):PHE:HB3	1.77	0.67
1:G:39:GLN:HB2	1:G:45:LEU:HD23	1.75	0.67

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:63:VAL:HG13	1:M:67:PHE:CD1	2.30	0.66
1:G:68:THR:OG1	1:G:81:GLU:OE2	2.10	0.66
2:I:150:LYS:HD3	2:I:195:GLN:HE21	1.59	0.66
1:H:200:HIS:ND1	1:H:203:SER:OG	2.26	0.66
1:M:166:PHE:HE1	1:M:181:VAL:HG12	1.60	0.66
1:U:50:ARG:HE	1:U:97:LYS:HZ3	1.44	0.66
2:V:55:PRO:HG2	2:V:58:ILE:HD13	1.77	0.66
1:U:67:PHE:CD2	1:U:82:MET:HA	2.30	0.66
1:G:210:LYS:NZ	1:G:212:GLU:OE1	2.21	0.65
1:G:100(J):GLU:O	3:G:302:HOH:O	2.15	0.65
1:H:165:THR:HG23	1:H:180:SER:HB2	1.77	0.65
2:V:188:GLN:O	2:V:192:HIS:ND1	2.30	0.65
1:U:59:TYR:CE1	1:U:69:ILE:HG13	2.28	0.64
1:U:97:LYS:HE2	1:U:100(J):GLU:CG	2.27	0.64
2:R:55:PRO:HB2	2:R:58:ILE:HD13	1.78	0.64
1:U:20:LEU:HD12	1:U:80:LEU:HD23	1.79	0.64
1:C:192:GLN:OE1	1:C:193:THR:N	2.29	0.64
2:I:24:ARG:HG3	2:I:24:ARG:HH11	1.63	0.64
2:N:62:PHE:CE2	2:N:75:ILE:HD11	2.32	0.64
1:U:94:ARG:O	1:U:101:GLN:N	2.31	0.63
2:N:89:SER:OG	3:N:301:HOH:O	2.15	0.63
2:L:14:ALA:HB3	2:L:17:GLN:HG3	1.79	0.63
1:M:122:PHE:CD2	2:N:124:GLU:HG2	2.34	0.63
1:Q:63:VAL:HG13	1:Q:67:PHE:HD1	1.63	0.63
2:D:195:GLN:HG2	2:D:204:GLU:HB2	1.82	0.62
2:N:37:GLN:HB2	2:N:47:LEU:HD11	1.82	0.62
1:U:142:VAL:HB	1:U:178:LEU:HG	1.82	0.62
1:M:122:PHE:HD2	2:N:124:GLU:HG2	1.63	0.62
1:U:33:TRP:CZ2	1:U:53:GLU:HG2	2.35	0.61
2:R:29:ARG:NH1	2:R:69:ASN:HB3	2.16	0.61
1:G:29:PHE:O	1:G:71:ARG:NH2	2.33	0.61
2:I:134:VAL:HG13	2:I:178:TYR:HE1	1.64	0.61
2:N:181:LEU:HG	2:N:185:GLN:HB2	1.82	0.61
1:U:100(J):GLU:HG3	2:V:91:ARG:NH2	2.16	0.61
1:C:89:TYR:OH	3:C:302:HOH:O	2.16	0.60
1:M:18:LEU:HD12	1:M:19:ARG:H	1.66	0.60
1:M:117:LYS:NZ	1:M:118:GLY:O	2.34	0.60
1:U:63:VAL:HG13	1:U:67:PHE:CD1	2.36	0.60
2:L:168:GLN:NE2	2:L:170:ASN:OD1	2.35	0.60
1:H:100(J):GLU:OE1	2:L:91:ARG:NH2	2.31	0.60
1:U:100(I):GLU:OE2	2:V:32:TYR:N	2.35	0.60

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:40:PRO:HB2	1:H:43:LYS:HG3	1.84	0.60
2:N:47:LEU:HD23	2:N:58:ILE:HD12	1.83	0.60
1:H:59:TYR:CE1	1:H:69:ILE:HD12	2.37	0.60
1:M:119:PRO:HB3	1:M:145:TYR:HB3	1.82	0.60
2:R:150:LYS:HE3	2:R:155:PRO:HD3	1.83	0.60
2:N:157:LYS:HD3	2:N:157:LYS:N	2.17	0.59
1:M:39:GLN:HB2	1:M:45:LEU:HD23	1.84	0.59
2:N:38:LYS:NZ	2:N:42:GLN:O	2.35	0.59
1:M:166:PHE:CE1	1:M:181:VAL:HG12	2.37	0.59
2:R:18:THR:HG22	2:R:76:THR:HA	1.83	0.59
2:I:80:ALA:HA	2:I:106:VAL:HG21	1.85	0.59
1:U:67:PHE:HD2	1:U:82:MET:HA	1.68	0.59
1:U:50:ARG:HE	1:U:97:LYS:NZ	2.01	0.59
2:V:12:SER:HB2	2:V:110:LEU:HD21	1.85	0.59
2:V:193:ARG:HD2	2:V:193:ARG:N	2.18	0.59
1:H:209:LYS:NZ	2:L:124:GLU:OE1	2.30	0.59
1:G:119:PRO:HB3	1:G:145:TYR:HB3	1.85	0.58
1:U:34:MET:HB3	1:U:78:LEU:HD22	1.84	0.58
1:C:210:LYS:HB3	1:U:204:ASN:HB3	1.85	0.58
1:U:98:TYR:HB3	1:U:100(H):GLY:HA3	1.86	0.58
2:L:37:GLN:HB2	2:L:47:LEU:HD11	1.86	0.58
1:H:98:TYR:HB3	1:H:100(H):GLY:HA3	1.86	0.58
1:U:96:GLY:O	1:U:97:LYS:HG3	2.04	0.58
2:L:46:LEU:HD11	2:L:49:TYR:HD1	1.68	0.57
1:M:59:TYR:HE1	1:M:69:ILE:HG13	1.69	0.57
1:Q:84:THR:HA	1:Q:111:VAL:HG13	1.86	0.57
1:U:29:PHE:O	1:U:71:ARG:NH2	2.37	0.57
1:G:66:ARG:HH21	1:G:83:ARG:HG2	1.69	0.57
2:L:67:SER:HB2	2:L:70:ARG:NH2	2.20	0.57
2:I:185:GLN:O	2:I:189:HIS:ND1	2.38	0.57
2:I:62:PHE:CE2	2:I:75:ILE:HD11	2.40	0.57
2:I:118:LEU:HD11	2:I:133:LEU:HD12	1.87	0.57
1:M:84:THR:HA	1:M:111:VAL:HG13	1.87	0.57
1:Q:67:PHE:CD2	1:Q:82:MET:HA	2.39	0.57
1:U:124:LEU:HB3	2:V:122:PHE:CD1	2.39	0.57
2:R:21:ILE:HG12	2:R:102:THR:HG21	1.88	0.56
3:H:301:HOH:O	2:L:95(B):ARG:O	2.17	0.56
2:D:139:ASP:OD1	2:D:170:ASN:ND2	2.39	0.56
2:R:37:GLN:HB2	2:R:47:LEU:HD11	1.87	0.56
2:I:172:LYS:HZ2	2:I:172:LYS:HB3	1.70	0.56
2:D:133:LEU:HB2	2:D:179:LEU:HB3	1.87	0.55

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:185:PRO:HG2	1:U:82(B):ASN:ND2	2.21	0.55
1:Q:18:LEU:HD12	1:Q:19:ARG:H	1.72	0.55
2:R:38:LYS:HB3	2:R:85:ASP:OD1	2.06	0.55
1:U:163:VAL:HG12	1:U:182:VAL:HG12	1.87	0.55
1:M:83:ARG:O	1:M:111:VAL:HG11	2.07	0.55
1:Q:170:LEU:HD13	1:Q:176:TYR:CE2	2.42	0.55
1:M:36:TRP:NE1	1:M:80:LEU:HB2	2.22	0.55
2:N:82:ASP:O	2:N:86:TYR:OH	2.17	0.54
1:G:61:GLU:HA	1:G:64:LYS:HE2	1.89	0.54
2:V:119:VAL:HG12	2:V:208:LYS:HD2	1.90	0.54
1:H:36:TRP:CE2	1:H:80:LEU:HB2	2.43	0.54
1:C:119:PRO:HB3	1:C:145:TYR:HB3	1.90	0.54
1:C:39:GLN:HB2	1:C:45:LEU:HD23	1.88	0.54
2:I:24:ARG:HG3	2:I:24:ARG:NH1	2.22	0.54
1:C:141:LEU:HD21	1:C:143:LYS:HD3	1.90	0.53
1:G:200:HIS:HD1	1:G:203:SER:HG	1.55	0.53
1:C:43:LYS:HE3	1:C:44:GLY:H	1.72	0.53
2:D:123:SER:HA	2:D:126:LEU:HD13	1.90	0.53
1:Q:145:TYR:OH	1:Q:178:LEU:HD23	2.09	0.53
1:G:138:LEU:HB2	1:G:211:VAL:HG11	1.90	0.53
1:M:88:GLY:O	1:M:109:VAL:N	2.40	0.53
1:G:71:ARG:HE	1:G:73:ASN:HD21	1.57	0.53
2:V:132:ASN:O	2:V:133:LYS:HE2	2.09	0.53
2:D:12:SER:HB2	2:D:107:LEU:HD11	1.90	0.53
1:G:147:PRO:HD2	1:G:202:PRO:HB3	1.91	0.53
2:R:148:ALA:HB3	2:R:195:GLN:HE21	1.73	0.53
1:M:200:HIS:CD2	1:M:202:PRO:HD2	2.44	0.52
1:Q:45:LEU:HD12	2:R:87:TYR:CD1	2.44	0.52
2:V:83:GLU:HG3	2:V:108:THR:HA	1.90	0.52
1:G:67:PHE:CZ	1:G:82:MET:HE3	2.44	0.52
1:U:82:MET:C	1:U:82(A):ASN:HD22	2.13	0.52
1:C:205:THR:HG22	1:U:209:LYS:HG2	1.92	0.52
1:H:31:ASN:HA	3:H:303:HOH:O	2.10	0.52
1:Q:63:VAL:HG13	1:Q:67:PHE:CD1	2.42	0.52
1:Q:6:GLU:OE1	1:Q:6:GLU:N	2.43	0.52
1:U:50:ARG:NH2	1:U:100(J):GLU:OE2	2.43	0.52
1:Q:100(I):GLU:CD	1:Q:100(I):GLU:H	2.13	0.52
2:L:46:LEU:HD11	2:L:49:TYR:CD1	2.45	0.52
1:U:67:PHE:CE2	1:U:82:MET:HB3	2.45	0.52
2:V:184:LEU:HD21	2:V:195:TYR:OH	2.10	0.52
2:N:133:LEU:HD12	2:N:179:LEU:HD23	1.92	0.51

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:36:TRP:CE2	1:M:80:LEU:HB2	2.45	0.51
2:V:119:VAL:HA	2:V:139:LEU:O	2.10	0.51
1:G:148:GLU:HB3	1:G:149:PRO:HA	1.92	0.51
2:N:18:THR:HA	2:N:75:ILE:O	2.10	0.51
1:H:166:PHE:HE1	1:H:181:VAL:HG12	1.75	0.51
1:Q:83:ARG:O	1:Q:111:VAL:HG11	2.10	0.51
1:Q:154:TRP:CH2	1:Q:196:CYS:HB3	2.46	0.51
1:U:154:TRP:CH2	1:U:196:CYS:HB3	2.46	0.51
2:V:119:VAL:O	2:V:208:LYS:NZ	2.23	0.51
1:Q:4:LEU:HD21	1:Q:27:PHE:HZ	1.76	0.51
1:H:126:PRO:HD2	1:H:213:PRO:HA	1.93	0.51
1:H:170:LEU:HD12	1:H:176:TYR:CZ	2.46	0.50
1:U:119:PRO:HB3	1:U:145:TYR:HB3	1.94	0.50
1:Q:35:THR:HG21	1:Q:100(L):PHE:CD1	2.46	0.50
2:R:38:LYS:NZ	2:R:39:LYS:O	2.43	0.50
1:H:138:LEU:HD21	1:H:194:TYR:CD1	2.46	0.50
2:L:36:TYR:CE2	2:L:46:LEU:HD23	2.46	0.50
1:H:6:GLU:OE2	1:H:91:PHE:HA	2.10	0.50
1:M:59:TYR:CE1	1:M:69:ILE:HG13	2.45	0.50
1:Q:119:PRO:HB3	1:Q:145:TYR:HB3	1.92	0.50
1:U:60:ALA:O	1:U:64:LYS:N	2.44	0.50
2:V:38:LYS:HD3	2:V:44:PRO:HG3	1.93	0.50
2:R:54:ARG:CZ	2:R:60:ASP:HA	2.42	0.50
1:U:33:TRP:NE1	1:U:53:GLU:OE1	2.44	0.50
1:Q:67:PHE:HD2	1:Q:82:MET:HA	1.77	0.50
1:C:122:PHE:HB2	1:C:141:LEU:HD22	1.94	0.50
1:Q:200:HIS:ND1	1:Q:203:SER:OG	2.33	0.49
2:N:184:GLU:OE1	2:N:188:SER:HB3	2.11	0.49
2:R:68:GLY:HA3	2:R:70:ARG:NH1	2.27	0.49
1:G:193:THR:HB	1:G:210:LYS:NZ	2.19	0.49
2:N:156:VAL:C	2:N:157:LYS:HD3	2.33	0.49
1:U:84:THR:HA	1:U:111:VAL:HB	1.95	0.49
2:V:115:ALA:HB3	2:V:144:TYR:N	2.26	0.49
1:G:93:ALA:HB1	1:G:100(L):PHE:HB3	1.94	0.49
2:I:38:LYS:HD3	2:I:44:PRO:HG3	1.95	0.49
2:I:195:GLN:OE1	2:I:204:GLU:HB3	2.12	0.49
1:M:166:PHE:CD2	2:N:176:SER:HB3	2.48	0.49
1:Q:141:LEU:HD12	2:R:134:VAL:HG21	1.95	0.49
2:V:6:GLN:HE21	2:V:102:GLY:HA3	1.78	0.49
2:V:188:GLN:HB3	2:V:192:HIS:HE1	1.77	0.49
1:H:56:SER:HB2	2:L:95(B):ARG:HH21	1.76	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:185:PRO:HG2	1:U:82(B):ASN:HD21	1.78	0.49
1:U:33:TRP:HZ2	1:U:53:GLU:HG2	1.78	0.49
2:V:13:VAL:HG21	2:V:19:VAL:HG22	1.95	0.49
1:Q:63:VAL:HG13	1:Q:67:PHE:HB2	1.95	0.48
1:U:22:CYS:HB3	1:U:78:LEU:HB3	1.94	0.48
2:V:151:ALA:HB3	2:V:198:GLN:HB2	1.95	0.48
1:H:192:GLN:HB3	1:H:194:TYR:CE2	2.49	0.48
1:M:3:ARG:HB2	1:M:3:ARG:CZ	2.43	0.48
2:L:116:VAL:O	2:L:205:LYS:HE3	2.14	0.48
2:D:111:LYS:HD2	2:D:111:LYS:O	2.13	0.48
2:R:6:GLN:HE21	2:R:99:GLY:HA3	1.78	0.48
2:L:60:ASP:OD1	2:L:60:ASP:N	2.45	0.48
2:D:32:TYR:OH	2:D:51:LYS:HE2	2.13	0.48
1:G:50:ARG:NH2	2:I:95(B):ARG:O	2.46	0.48
2:N:92:ASP:OD1	2:N:92:ASP:N	2.44	0.48
1:G:99:TYR:CE1	1:G:100(D):GLY:HA2	2.49	0.48
1:M:13:LYS:HG3	1:M:14:PRO:HD2	1.95	0.48
1:C:141:LEU:HD12	2:D:134:VAL:HG21	1.95	0.48
1:M:87:THR:HG23	1:M:110:ILE:HA	1.96	0.48
1:Q:186:SER:HA	1:Q:189:LEU:HG	1.95	0.48
1:U:181:VAL:HG21	2:V:139:LEU:CD1	2.40	0.48
2:I:133:LEU:HB2	2:I:179:LEU:HB3	1.96	0.48
2:N:143:GLY:HA3	2:N:173:TYR:CD2	2.49	0.48
1:G:150:VAL:HG12	1:G:200:HIS:CD2	2.48	0.48
1:Q:53:GLU:N	1:Q:53:GLU:OE2	2.47	0.48
2:L:39:LYS:HB2	2:L:42:GLN:HE21	1.79	0.47
2:L:137:ILE:HG12	2:L:196:VAL:HG21	1.96	0.47
1:Q:141:LEU:CD2	1:Q:143:LYS:HG3	2.37	0.47
1:Q:159:LEU:HD21	1:Q:182:VAL:HG11	1.96	0.47
2:R:137:ILE:HD12	2:R:175:ALA:HB3	1.96	0.47
1:H:56:SER:HB2	2:L:95(B):ARG:NH2	2.29	0.47
1:G:100:ASP:O	1:G:100(A):PHE:HB3	2.14	0.47
1:G:82(B):ASN:OD1	1:G:83:ARG:NH2	2.42	0.47
2:L:61:ARG:HB2	2:L:76:THR:O	2.14	0.47
1:G:8:GLY:O	1:G:18:LEU:HD11	2.15	0.47
2:I:134:VAL:HG13	2:I:178:TYR:CE1	2.48	0.47
2:D:181:LEU:HD11	2:D:192:TYR:CZ	2.50	0.47
1:H:154:TRP:CH2	1:H:196:CYS:HB3	2.49	0.47
2:L:126:LEU:HD21	2:L:186:TRP:HD1	1.79	0.47
1:C:207:VAL:HG13	1:U:207:VAL:HG22	1.97	0.47
2:N:48:PHE:CE2	2:N:54:ARG:HB2	2.49	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:144:ASP:OD1	1:U:175:LEU:HG	2.14	0.47
1:H:204:ASN:HB3	1:Q:210:LYS:HG3	1.96	0.47
2:D:122:SER:O	2:D:126:LEU:HD12	2.15	0.47
1:C:184:VAL:HG11	1:C:194:TYR:OH	2.14	0.47
2:V:193:ARG:HD2	2:V:193:ARG:H	1.79	0.47
1:G:2:VAL:HG11	1:G:102:ASP:OD2	2.14	0.47
1:G:20:LEU:HD21	1:G:82:MET:SD	2.55	0.47
1:Q:94:ARG:HD3	1:Q:101:GLN:NE2	2.24	0.47
2:R:195:GLN:OE1	2:R:197:THR:HG23	2.14	0.47
1:C:141:LEU:HD21	1:C:143:LYS:HG3	1.97	0.46
1:H:200:HIS:NE2	1:H:202:PRO:HG2	2.30	0.46
1:U:18:LEU:HD12	1:U:19:ARG:H	1.80	0.46
1:U:87:THR:HA	1:U:88:GLY:HA2	1.64	0.46
1:C:87:THR:HA	1:C:88:GLY:HA2	1.66	0.46
1:G:87:THR:HA	1:G:88:GLY:HA2	1.64	0.46
1:M:3:ARG:HB2	1:M:3:ARG:NH1	2.29	0.46
2:V:198:GLN:OE1	2:V:207:GLU:HB3	2.15	0.46
1:H:123:PRO:HD3	1:H:209:LYS:HE2	1.97	0.46
2:L:24:ARG:HE	2:L:70:ARG:HG2	1.80	0.46
2:L:48:PHE:CE2	2:L:52:ASN:HA	2.50	0.46
1:C:163:VAL:HG12	1:C:182:VAL:HG22	1.97	0.46
1:Q:87:THR:HG23	1:Q:110:ILE:HA	1.97	0.46
2:L:122:SER:O	2:L:126:LEU:HD12	2.16	0.46
1:G:108:LEU:HD12	1:G:109:VAL:N	2.30	0.46
1:M:50:ARG:HH11	1:M:52:THR:HG23	1.79	0.46
1:Q:100(I):GLU:OE1	2:R:32:TYR:N	2.49	0.46
2:V:153:LYS:HB3	2:V:196:SER:HB2	1.98	0.46
1:C:204:ASN:ND2	1:U:210:LYS:HE2	2.31	0.46
1:M:33:TRP:CE2	1:M:52:THR:HG22	2.50	0.46
1:Q:195:ILE:HD13	1:Q:195:ILE:HA	1.82	0.46
1:U:145:TYR:CZ	1:U:178:LEU:HD23	2.50	0.46
2:L:49:TYR:O	2:L:53:ASN:HB2	2.16	0.46
1:G:34:MET:HB3	1:G:78:LEU:HD22	1.97	0.46
1:Q:33:TRP:NE1	1:Q:53:GLU:OE1	2.47	0.46
2:R:4:LEU:HD12	2:R:4:LEU:H	1.80	0.46
1:U:82:MET:HE1	1:U:90:TYR:CZ	2.51	0.46
1:H:96:GLY:HA3	1:H:101:GLN:HE21	1.81	0.45
2:L:135:CYS:HB2	2:L:149:TRP:CH2	2.51	0.45
1:M:34:MET:HB3	1:M:78:LEU:HD13	1.98	0.45
1:Q:138:LEU:HD13	1:Q:211:VAL:HG11	1.98	0.45
1:Q:150:VAL:HG23	1:Q:200:HIS:HD2	1.81	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:151:THR:HG23	1:Q:199:ASN:HB3	1.98	0.45
2:N:195:GLN:HG2	2:N:204:GLU:HB2	1.98	0.45
1:Q:154:TRP:CZ3	1:Q:196:CYS:HB3	2.51	0.45
1:U:171:GLN:OE1	1:U:177:SER:OG	2.33	0.45
1:G:84:THR:HA	1:G:111:VAL:HG11	1.99	0.45
1:G:200:HIS:CD2	1:G:202:PRO:HD2	2.52	0.45
2:L:3:GLU:N	2:L:3:GLU:OE1	2.50	0.45
1:G:200:HIS:ND1	1:G:203:SER:OG	2.44	0.45
2:I:18:THR:HA	2:I:75:ILE:O	2.17	0.45
2:N:135:CYS:HB2	2:N:149:TRP:CH2	2.51	0.45
1:U:33:TRP:HE3	1:U:97:LYS:NZ	2.06	0.45
1:M:200:HIS:HB3	1:M:205:THR:OG1	2.16	0.45
2:D:181:LEU:HD13	2:D:185:GLN:HB2	1.98	0.45
1:M:29:PHE:O	1:M:71:ARG:NH2	2.49	0.45
1:M:53:GLU:N	1:M:53:GLU:OE1	2.50	0.45
1:U:8:GLY:O	1:U:18:LEU:HD11	2.16	0.45
1:H:200:HIS:CE1	1:H:203:SER:HG	2.30	0.45
2:R:134:VAL:HG22	2:R:178:TYR:CD1	2.52	0.45
2:R:140:PHE:CE1	2:R:145:VAL:HG13	2.51	0.45
1:U:214:LYS:HE2	1:U:214:LYS:HB3	1.78	0.45
1:H:39:GLN:HB2	1:H:45:LEU:HD23	1.98	0.45
1:H:204:ASN:HB3	1:Q:210:LYS:CG	2.47	0.45
1:U:37:VAL:HG11	1:U:45:LEU:HD13	1.97	0.45
1:U:146:PHE:HA	1:U:147:PRO:HA	1.78	0.45
2:V:54:ARG:HD2	2:V:58:ILE:HG22	1.99	0.45
2:D:135:CYS:HB2	2:D:149:TRP:CH2	2.52	0.45
1:M:146:PHE:HB2	1:M:175:LEU:HD22	1.98	0.45
2:R:85:ASP:HB3	2:R:103:LYS:HD3	1.99	0.45
2:N:4:LEU:HD22	2:N:23:CYS:SG	2.58	0.44
2:N:109:GLN:NE2	2:N:171:ASN:HB3	2.32	0.44
1:Q:143:LYS:HD2	2:R:132:THR:HG21	1.98	0.44
1:U:97:LYS:CE	1:U:100(J):GLU:HG2	2.36	0.44
1:U:123:PRO:HG3	1:U:209:LYS:NZ	2.31	0.44
1:H:121:VAL:HB	1:H:207:VAL:HG11	2.00	0.44
1:H:206:LYS:HB3	1:H:206:LYS:HE3	1.80	0.44
1:M:124:LEU:HD12	1:M:140:CYS:N	2.33	0.44
2:N:51:LYS:NZ	3:N:302:HOH:O	2.21	0.44
1:Q:11:LEU:HA	1:Q:110:ILE:O	2.17	0.44
1:Q:66:ARG:NH2	1:Q:86:ASP:OD2	2.50	0.44
1:U:145:TYR:O	1:U:176:TYR:HB2	2.18	0.44
1:C:29:PHE:O	1:C:71:ARG:NH2	2.51	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:167:LYS:HE2	2:R:167:LYS:HB3	1.56	0.44
1:M:52:THR:OG1	1:M:56:SER:N	2.50	0.44
1:Q:4:LEU:HD21	1:Q:27:PHE:CZ	2.53	0.44
2:R:35:TRP:CH2	2:R:88:CYS:HB3	2.52	0.44
1:G:59:TYR:HB2	1:G:64:LYS:HG3	1.99	0.44
1:G:142:VAL:HB	1:G:178:LEU:HD12	2.00	0.44
1:M:86:ASP:N	1:M:86:ASP:OD1	2.48	0.44
1:Q:142:VAL:HB	1:Q:178:LEU:HG	1.98	0.44
2:V:83:GLU:CG	2:V:108:THR:HA	2.48	0.44
2:I:109:GLN:HB2	2:I:141:TYR:CE2	2.53	0.44
1:Q:100(J):GLU:HG3	2:R:91:ARG:NH1	2.33	0.44
1:H:87:THR:HA	1:H:88:GLY:HA2	1.72	0.44
1:M:147:PRO:O	1:M:200:HIS:NE2	2.37	0.44
1:Q:2:VAL:C	1:Q:3:ARG:HD3	2.37	0.44
2:V:192:HIS:HD1	2:V:195:TYR:HH	1.53	0.44
1:C:143:LYS:HB3	1:C:143:LYS:HE2	1.72	0.43
1:U:166:PHE:CD2	2:V:179:SER:HB3	2.52	0.43
1:G:96:GLY:HA3	1:G:100(K):TYR:CZ	2.53	0.43
2:L:195:GLN:CG	2:L:204:GLU:HB3	2.48	0.43
1:U:110:ILE:HD13	1:U:176:TYR:OH	2.18	0.43
2:L:36:TYR:CZ	2:L:46:LEU:HD23	2.53	0.43
2:R:140:PHE:HZ	2:R:165:PRO:HB3	1.83	0.43
1:H:119:PRO:HB3	1:H:145:TYR:HB3	2.00	0.43
1:Q:1:GLU:HA	1:Q:3:ARG:NH1	2.33	0.43
1:U:40:PRO:HB2	1:U:43:LYS:HB2	2.01	0.43
1:U:50:ARG:HH21	1:U:100(J):GLU:CD	2.22	0.43
1:C:19:ARG:NH1	3:C:309:HOH:O	2.51	0.43
1:Q:82:MET:HE3	1:Q:109:VAL:HG21	2.00	0.43
1:H:94:ARG:NH1	1:H:102:ASP:OD2	2.51	0.43
1:M:138:LEU:O	1:M:182:VAL:HG22	2.19	0.43
1:G:51:ILE:HG13	1:G:57:VAL:HG22	1.99	0.43
2:N:125:GLU:OE2	2:N:132:THR:HG23	2.19	0.43
1:C:14:PRO:HD2	1:C:113:SER:HB3	2.00	0.43
2:R:114:PRO:HB3	2:R:140:PHE:HB3	2.00	0.43
1:U:38:ARG:NE	1:U:46:GLU:OE1	2.31	0.43
1:C:82(B):ASN:O	1:C:83:ARG:HD3	2.18	0.42
1:G:126:PRO:HD3	1:G:138:LEU:HB3	2.00	0.42
1:U:34:MET:O	1:U:50:ARG:HG2	2.19	0.42
1:H:138:LEU:HD21	1:H:194:TYR:HD1	1.84	0.42
1:H:205:THR:HG22	1:Q:209:LYS:HE2	2.00	0.42
2:N:149:TRP:HE1	2:N:177:SER:HG	1.67	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:34:MET:O	1:H:50:ARG:HG2	2.20	0.42
1:H:53:GLU:HB3	1:G:100(A):PHE:HE1	1.84	0.42
1:C:88:GLY:HA2	1:C:109:VAL:O	2.19	0.42
1:M:144:ASP:HA	1:M:175:LEU:HB3	2.01	0.42
1:M:166:PHE:CD1	1:M:166:PHE:N	2.87	0.42
1:Q:36:TRP:CE2	1:Q:80:LEU:HB2	2.55	0.42
2:R:6:GLN:NE2	2:R:88:CYS:SG	2.92	0.42
2:L:32:TYR:OH	2:L:51:LYS:HD2	2.20	0.42
1:C:43:LYS:HA	1:C:43:LYS:HD2	1.93	0.42
1:Q:30:ASP:O	1:Q:52(B):PRO:HD3	2.20	0.42
1:Q:195:ILE:HD13	1:Q:210:LYS:HA	2.02	0.42
1:C:84:THR:HA	1:C:111:VAL:HB	2.01	0.42
1:G:59:TYR:HE1	1:G:69:ILE:HG13	1.83	0.42
2:I:133:LEU:HD23	2:I:181:LEU:HD23	2.01	0.42
1:M:67:PHE:CE2	1:M:82:MET:HE3	2.54	0.42
2:N:199:GLU:OE2	2:N:199:GLU:HA	2.19	0.42
1:Q:108:LEU:HD12	1:Q:109:VAL:N	2.34	0.42
1:G:51:ILE:HD13	1:G:71:ARG:HD2	2.02	0.42
2:V:117:PRO:HD3	2:V:201:HIS:CD2	2.55	0.42
2:V:193:ARG:H	2:V:193:ARG:CD	2.32	0.42
2:L:195:GLN:HG2	2:L:204:GLU:HB3	2.01	0.42
1:G:145:TYR:CE1	1:G:150:VAL:HG13	2.55	0.42
1:M:87:THR:HA	1:M:88:GLY:HA2	1.64	0.42
1:U:124:LEU:HD21	1:U:141:LEU:HB2	2.02	0.42
1:C:169:VAL:HB	2:D:163:THR:HG22	2.02	0.42
2:I:145:VAL:HG12	2:I:198:HIS:HB2	2.01	0.41
1:Q:87:THR:HA	1:Q:88:GLY:HA2	1.67	0.41
1:Q:170:LEU:HD13	1:Q:176:TYR:HE2	1.85	0.41
1:U:5:VAL:O	1:U:22:CYS:HA	2.20	0.41
1:H:154:TRP:CZ3	1:H:196:CYS:HB3	2.55	0.41
1:C:82(B):ASN:OD1	1:C:83:ARG:NH1	2.53	0.41
1:U:4:LEU:HD12	1:U:103:TRP:C	2.39	0.41
2:V:193:ARG:N	2:V:193:ARG:CD	2.83	0.41
1:H:112:SER:HB3	1:H:146:PHE:HE2	1.85	0.41
2:D:182:THR:OG1	2:D:185:GLN:HG3	2.20	0.41
1:M:146:PHE:HA	1:M:147:PRO:HA	1.80	0.41
1:H:112:SER:CB	1:H:146:PHE:HE2	2.33	0.41
1:M:75:LYS:HB2	1:M:77:THR:HG23	2.03	0.41
1:Q:50:ARG:HB3	1:Q:50:ARG:CZ	2.50	0.41
2:N:32:TYR:OH	2:N:51:LYS:HE2	2.21	0.41
1:Q:16:GLY:O	1:Q:82(C):VAL:HG23	2.20	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:26:ASP:O	2:R:29:ARG:HG3	2.20	0.41
1:U:143:LYS:HZ2	1:U:144:ASP:CG	2.24	0.41
1:C:16:GLY:O	1:C:82(C):VAL:HG23	2.20	0.41
1:C:59:TYR:CE2	1:C:69:ILE:HD12	2.55	0.41
2:D:37:GLN:HB2	2:D:47:LEU:HD11	2.02	0.41
1:G:84:THR:HA	1:G:111:VAL:CG1	2.50	0.41
1:M:4:LEU:HA	1:M:4:LEU:HD23	1.80	0.41
1:M:72:ASP:OD1	1:M:75:LYS:HG3	2.21	0.41
1:U:18:LEU:HD12	1:U:19:ARG:N	2.36	0.41
2:L:136:LEU:HD23	2:L:136:LEU:HA	1.91	0.41
2:N:47:LEU:HD22	2:N:62:PHE:CE2	2.56	0.41
2:N:136:LEU:HD23	2:N:136:LEU:HA	1.68	0.41
2:L:92:ASP:OD1	2:L:92:ASP:N	2.48	0.41
1:C:83:ARG:HD3	1:C:83:ARG:N	2.36	0.41
1:C:93:ALA:HB1	1:C:100(L):PHE:HB3	2.02	0.41
1:C:204:ASN:HD22	1:U:210:LYS:HE2	1.86	0.41
2:D:180:SER:O	2:D:181:LEU:HD23	2.20	0.41
1:G:119:PRO:HB2	1:G:142:VAL:HG13	2.03	0.41
1:Q:72:ASP:OD1	1:Q:75:LYS:N	2.48	0.41
1:Q:82:MET:CE	1:Q:109:VAL:HG21	2.51	0.41
2:R:95(B):ARG:H	2:R:95(B):ARG:HG2	1.56	0.41
2:L:109:GLN:OE1	2:L:171:ASN:HB3	2.21	0.41
1:G:43:LYS:HZ3	1:G:43:LYS:HB2	1.86	0.41
1:G:152:VAL:HG11	1:G:180:SER:OG	2.20	0.41
1:Q:40:PRO:CB	1:Q:43:LYS:HD2	2.47	0.41
2:V:18:THR:HA	2:V:75:ILE:O	2.21	0.41
1:H:101:GLN:H	1:H:101:GLN:HG3	1.64	0.40
1:H:126:PRO:HG3	1:H:138:LEU:CD2	2.51	0.40
2:I:126:LEU:HD11	2:I:186:TRP:CD1	2.56	0.40
1:Q:38:ARG:NE	1:Q:46:GLU:OE1	2.53	0.40
2:R:181:LEU:HD11	2:R:192:TYR:OH	2.21	0.40
1:U:124:LEU:HD12	1:U:139:GLY:C	2.42	0.40
2:V:83:GLU:HG2	2:V:107:LEU:O	2.20	0.40
1:H:117:LYS:HE2	1:H:117:LYS:HB3	1.82	0.40
1:C:43:LYS:CE	1:C:44:GLY:H	2.33	0.40
1:G:12:VAL:O	1:G:111:VAL:HA	2.21	0.40
1:Q:12:VAL:O	1:Q:111:VAL:HA	2.22	0.40
1:U:36:TRP:CZ3	1:U:92:CYS:HB3	2.56	0.40
1:U:50:ARG:NE	1:U:97:LYS:NZ	2.69	0.40
1:H:51:ILE:HD13	1:H:71:ARG:HD2	2.02	0.40
1:H:150:VAL:HG21	1:H:178:LEU:HD21	2.03	0.40

*Continued on next page...*



Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:50:ARG:HG2	1:C:51:ILE:N	2.35	0.40
1:C:20:LEU:HD12	1:C:80:LEU:HD23	2.02	0.40
1:G:75:LYS:HB2	1:G:75:LYS:HE2	1.69	0.40
1:G:147:PRO:HD2	1:G:202:PRO:CB	2.49	0.40
1:Q:100(I):GLU:OE2	2:R:32:TYR:HB2	2.21	0.40
2:V:117:PRO:HA	2:V:143:PHE:HB3	2.03	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	221/233 (95%)	216 (98%)	5 (2%)	0	100	100
1	G	220/233 (94%)	214 (97%)	6 (3%)	0	100	100
1	H	220/233 (94%)	216 (98%)	4 (2%)	0	100	100
1	M	220/233 (94%)	218 (99%)	2 (1%)	0	100	100
1	Q	219/233 (94%)	217 (99%)	2 (1%)	0	100	100
1	U	220/233 (94%)	216 (98%)	4 (2%)	0	100	100
2	D	207/215 (96%)	203 (98%)	4 (2%)	0	100	100
2	I	208/215 (97%)	198 (95%)	10 (5%)	0	100	100
2	L	207/215 (96%)	201 (97%)	6 (3%)	0	100	100
2	N	207/215 (96%)	202 (98%)	5 (2%)	0	100	100
2	R	207/215 (96%)	204 (99%)	3 (1%)	0	100	100
2	V	207/215 (96%)	203 (98%)	4 (2%)	0	100	100
All	All	2563/2688 (95%)	2508 (98%)	55 (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	188/194 (97%)	182 (97%)	6 (3%)	39	59
1	G	186/194 (96%)	181 (97%)	5 (3%)	44	65
1	H	186/194 (96%)	183 (98%)	3 (2%)	62	79
1	M	183/194 (94%)	175 (96%)	8 (4%)	28	45
1	Q	186/194 (96%)	179 (96%)	7 (4%)	33	51
1	U	184/194 (95%)	175 (95%)	9 (5%)	25	40
2	D	174/180 (97%)	168 (97%)	6 (3%)	37	56
2	I	175/180 (97%)	173 (99%)	2 (1%)	73	87
2	L	174/180 (97%)	172 (99%)	2 (1%)	73	87
2	N	175/180 (97%)	171 (98%)	4 (2%)	50	70
2	R	167/180 (93%)	157 (94%)	10 (6%)	19	31
2	V	172/180 (96%)	165 (96%)	7 (4%)	30	48
All	All	2150/2244 (96%)	2081 (97%)	69 (3%)	39	59

All (69) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	97	LYS
1	H	146	PHE
1	H	179	SER
2	L	119	PHE
2	L	155	PRO
1	C	23	SER
1	C	50	ARG
1	C	84	THR
1	C	97	LYS
1	C	197	ASN
1	C	208	ASP
2	D	56	SER
2	D	111	LYS
2	D	115	SER

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	D	154	SER
2	D	168	GLN
2	D	187	LYS
1	G	73	ASN
1	G	97	LYS
1	G	100(A)	PHE
1	G	178	LEU
1	G	209	LYS
2	I	5	THR
2	I	6	GLN
1	M	23	SER
1	M	30	ASP
1	M	86	ASP
1	M	97	LYS
1	M	100(A)	PHE
1	M	112	SER
1	M	191	THR
1	M	201	LYS
2	N	26	ASP
2	N	103	LYS
2	N	157	LYS
2	N	171	ASN
1	Q	3	ARG
1	Q	50	ARG
1	Q	97	LYS
1	Q	98	TYR
1	Q	188	SER
1	Q	193	THR
1	Q	204	ASN
2	R	16	LYS
2	R	17	GLN
2	R	56	SER
2	R	70	ARG
2	R	111	LYS
2	R	137	ILE
2	R	141	TYR
2	R	173	TYR
2	R	195	GLN
2	R	198	HIS
1	U	43	LYS
1	U	53	GLU
1	U	73	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	U	76	ASN
1	U	81	GLU
1	U	94	ARG
1	U	191	THR
1	U	199	ASN
1	U	214	LYS
2	V	26	ASP
2	V	53	ASN
2	V	70	ARG
2	V	95(B)	ARG
2	V	106	LYS
2	V	122	PHE
2	V	190	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	164	HIS
2	L	42	GLN
2	D	189	HIS
1	G	73	ASN
2	I	195	GLN
1	M	164	HIS
2	N	171	ASN
2	N	189	HIS
1	Q	101	GLN
1	Q	164	HIS
2	R	6	GLN
1	U	82(A)	ASN
2	V	6	GLN
2	V	112	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates [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

### 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	225/233 (96%)	0.25	7 (3%) 49 47	49, 84, 114, 128	0
1	G	224/233 (96%)	0.49	22 (9%) 7 7	61, 106, 140, 161	0
1	H	224/233 (96%)	0.27	17 (7%) 13 12	52, 89, 122, 152	0
1	M	224/233 (96%)	0.52	24 (10%) 6 5	59, 104, 130, 148	0
1	Q	223/233 (95%)	0.46	19 (8%) 10 10	80, 104, 130, 153	0
1	U	224/233 (96%)	0.65	34 (15%) 2 1	81, 110, 140, 159	0
2	D	209/215 (97%)	-0.08	5 (2%) 59 57	54, 85, 118, 140	0
2	I	210/215 (97%)	0.10	12 (5%) 23 22	49, 88, 142, 169	0
2	L	209/215 (97%)	-0.00	6 (2%) 51 50	50, 84, 129, 147	0
2	N	209/215 (97%)	0.14	10 (4%) 30 29	51, 91, 133, 159	0
2	R	209/215 (97%)	0.74	30 (14%) 2 2	88, 119, 151, 174	0
2	V	209/215 (97%)	0.59	28 (13%) 3 2	86, 114, 148, 165	0
All	All	2599/2688 (96%)	0.35	214 (8%) 11 10	49, 100, 138, 174	0

All (214) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	N	207	VAL	6.0
1	U	189	LEU	5.8
2	N	187	LYS	4.8
2	R	204	GLU	4.5
2	V	159	VAL	4.5
1	M	160	THR	4.4
2	R	146	THR	4.4
2	V	48	PHE	4.3
2	V	210	VAL	4.3
2	R	203	VAL	4.2
2	V	206	VAL	4.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	R	23	CYS	4.1
1	H	112	SER	4.1
1	Q	189	LEU	4.1
1	G	1	GLU	4.1
2	I	184	GLU	4.0
2	R	62	PHE	4.0
2	V	204	SER	4.0
1	U	82(B)	ASN	4.0
2	N	192	TYR	3.9
2	I	153	SER	3.9
2	I	207	VAL	3.9
2	I	181	LEU	3.8
2	R	13	VAL	3.8
2	V	190	LYS	3.8
2	R	79	GLN	3.8
2	I	155	PRO	3.8
1	G	110	ILE	3.7
2	R	159	GLY	3.7
2	V	19	VAL	3.7
1	U	100(A)	PHE	3.6
2	V	195	TYR	3.6
1	G	159	LEU	3.6
1	C	189	LEU	3.5
1	U	98	TYR	3.5
2	V	13	VAL	3.5
1	Q	173	SER	3.5
2	R	147	VAL	3.5
1	Q	61	GLU	3.5
2	V	161	ALA	3.5
2	I	151	ALA	3.4
1	U	49	GLY	3.4
1	Q	100(A)	PHE	3.4
1	M	35	THR	3.3
1	G	193	THR	3.3
2	R	151	ALA	3.3
2	L	190	ARG	3.3
1	G	184	VAL	3.3
2	R	199	GLU	3.3
1	G	158	ALA	3.2
1	Q	35	THR	3.2
1	G	176	TYR	3.2
2	V	47	LEU	3.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	H	195	ILE	3.2
1	U	75	LYS	3.2
1	G	111	VAL	3.2
1	M	1	GLU	3.2
2	R	202	THR	3.2
1	M	135	THR	3.2
2	V	49	TYR	3.1
1	Q	141	LEU	3.1
1	G	196	CYS	3.1
1	H	193	THR	3.1
1	M	33	TRP	3.1
2	R	106	VAL	3.1
1	U	10	GLY	3.1
1	U	100(J)	GLU	3.1
2	V	160	LYS	3.1
2	N	151	ALA	3.1
2	R	78	ALA	3.1
1	M	120	SER	3.1
1	U	112	SER	3.1
1	U	110	ILE	3.0
1	M	95	THR	3.0
1	M	188	SER	3.0
1	U	35	THR	3.0
1	U	95	THR	3.0
2	R	112	ALA	3.0
1	G	210	LYS	3.0
1	U	67	PHE	3.0
2	N	152	ASP	3.0
1	U	188	SER	3.0
1	G	175	LEU	3.0
1	M	138	LEU	3.0
2	N	131	ALA	3.0
1	M	109	VAL	2.9
2	R	34	SER	2.9
2	L	157	LYS	2.9
2	R	66	ALA	2.9
2	D	156	VAL	2.9
1	C	120	SER	2.9
1	M	36	TRP	2.9
2	N	203	VAL	2.8
1	G	101	GLN	2.8
1	Q	186	SER	2.8

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	U	51	ILE	2.8
2	R	158	ALA	2.8
2	I	183	PRO	2.8
1	U	100(K)	TYR	2.7
2	R	192	TYR	2.7
1	H	35	THR	2.7
2	I	152	ASP	2.7
2	V	162	GLY	2.7
2	V	56	SER	2.7
1	Q	103	TRP	2.7
1	C	92	CYS	2.7
2	I	2	SER	2.7
1	C	98	TYR	2.7
2	R	107	LEU	2.7
2	R	35	TRP	2.7
1	Q	1	GLU	2.6
2	N	155	PRO	2.6
1	U	24	ALA	2.6
1	Q	29	PHE	2.6
2	R	100	GLY	2.6
1	H	37	VAL	2.6
1	U	144	ASP	2.6
2	L	158	ALA	2.6
1	C	195	ILE	2.6
2	R	200	GLY	2.6
1	U	140	CYS	2.5
1	U	213	PRO	2.5
1	U	48	VAL	2.5
1	G	35	THR	2.5
1	M	166	PHE	2.5
1	Q	140	CYS	2.5
1	C	112	SER	2.5
1	U	212	GLU	2.5
1	H	49	GLY	2.5
1	G	190	GLY	2.5
1	H	189	LEU	2.5
1	U	33	TRP	2.5
1	U	100(G)	ALA	2.5
2	V	136	LEU	2.4
1	G	194	TYR	2.4
1	H	69	ILE	2.4
1	G	95	THR	2.4

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	U	194	TYR	2.4
2	V	179	SER	2.4
1	M	75	LYS	2.4
2	I	127	GLN	2.4
2	V	205	THR	2.4
1	U	192	GLN	2.4
1	H	34	MET	2.4
1	H	140	CYS	2.4
1	M	177	SER	2.4
2	V	107	LEU	2.4
1	M	110	ILE	2.4
2	V	21	ILE	2.4
1	G	191	THR	2.4
1	U	11	LEU	2.4
1	U	97	LYS	2.3
1	M	51	ILE	2.3
2	N	150	LYS	2.3
2	V	75	ILE	2.3
2	L	181	LEU	2.3
1	G	93	ALA	2.3
1	G	140	CYS	2.3
2	R	113	ALA	2.3
2	I	187	LYS	2.3
1	Q	179	SER	2.3
1	U	8	GLY	2.3
1	Q	138	LEU	2.3
2	R	160	VAL	2.2
1	H	159	LEU	2.2
2	V	28	LEU	2.2
1	Q	49	GLY	2.2
2	R	145	VAL	2.2
1	H	114	ALA	2.2
2	D	206	THR	2.2
2	D	157	LYS	2.2
1	H	96	GLY	2.2
2	R	89	SER	2.2
2	R	15	LEU	2.2
1	U	50	ARG	2.2
2	V	24	ARG	2.2
2	V	187	GLU	2.2
2	I	118	LEU	2.2
1	Q	100(J)	GLU	2.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	M	189	LEU	2.1
1	Q	146	PHE	2.1
2	N	136	LEU	2.1
1	C	34	MET	2.1
1	M	121	VAL	2.1
1	M	93	ALA	2.1
1	M	123	PRO	2.1
1	H	100(L)	PHE	2.1
1	G	33	TRP	2.1
1	Q	187	SER	2.1
1	H	95	THR	2.1
1	M	48	VAL	2.1
1	M	145	TYR	2.1
2	V	32	TYR	2.1
2	V	181	TYR	2.1
1	G	189	LEU	2.1
2	R	46	LEU	2.1
2	L	200	GLY	2.1
2	D	202	THR	2.1
2	D	192	TYR	2.1
2	V	180	SER	2.1
1	U	3	ARG	2.1
1	U	113	SER	2.0
1	Q	124	LEU	2.0
2	R	174	ALA	2.0
2	L	189	HIS	2.0
1	U	187	SER	2.0
1	Q	100(K)	TYR	2.0
1	H	191	THR	2.0
2	V	138	CYS	2.0
1	H	198	VAL	2.0
1	M	37	VAL	2.0
1	U	9	GLY	2.0
1	G	45	LEU	2.0
1	M	141	LEU	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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.