



# Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 05:35 am BST

PDB ID : 5TLA  
Title : Crystal structure of mouse ISG15  
Authors : Goodwin, O.Y.; Dzimianski, J.V.; Daczkowski, C.M.; Pegan, S.D.  
Deposited on : 2016-10-10  
Resolution : 3.24 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	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

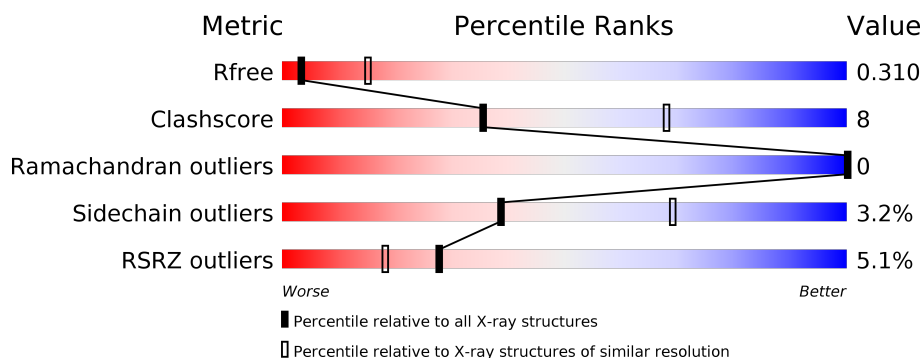
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.24 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	1619 (3.28-3.20)
Clashscore	141614	1755 (3.28-3.20)
Ramachandran outliers	138981	1728 (3.28-3.20)
Sidechain outliers	138945	1727 (3.28-3.20)
RSRZ outliers	127900	1567 (3.28-3.20)

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	151	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 25%, green 74%);"></div> <div style="display: flex; justify-content: space-between; margin-top: 2px;"> <span>%</span> <span>74%</span> <span>25%</span> <span>.</span> </div> </div>
1	B	151	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 3%, orange 1%, yellow 22%, green 76%);"></div> <div style="display: flex; justify-content: space-between; margin-top: 2px;"> <span>3%</span> <span>76%</span> <span>22%</span> <span>.</span> </div> </div>
1	C	151	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 25%, green 74%);"></div> <div style="display: flex; justify-content: space-between; margin-top: 2px;"> <span>%</span> <span>74%</span> <span>25%</span> <span>..</span> </div> </div>
1	D	151	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 5%, orange 1%, yellow 19%, green 76%, grey 5%);"></div> <div style="display: flex; justify-content: space-between; margin-top: 2px;"> <span>5%</span> <span>76%</span> <span>19%</span> <span>5%</span> </div> </div>
1	E	151	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 19%, green 79%);"></div> <div style="display: flex; justify-content: space-between; margin-top: 2px;"> <span>%</span> <span>79%</span> <span>19%</span> <span>..</span> </div> </div>
1	F	151	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 3%, orange 1%, yellow 23%, green 76%);"></div> <div style="display: flex; justify-content: space-between; margin-top: 2px;"> <span>3%</span> <span>76%</span> <span>23%</span> <span>.</span> </div> </div>

*Continued on next page...*

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	G	151	<div><div></div><div>5%</div><div>78%</div><div>17%</div><div>5%</div></div>
1	H	151	<div><div></div><div>11%</div><div>77%</div><div>14%</div><div>6%</div></div>
1	I	151	<div><div></div><div>13%</div><div>66%</div><div>24%</div><div>11%</div></div>
1	J	151	<div><div></div><div>7%</div><div>77%</div><div>15%</div><div>7%</div></div>

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 11491 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 Ubiquitin-like protein ISG15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	151	Total	C	N	O	S	0	0	0
			1190	753	206	225	6			
1	B	151	Total	C	N	O	S	0	0	0
			1190	753	206	225	6			
1	C	150	Total	C	N	O	S	0	0	0
			1180	747	203	224	6			
1	D	144	Total	C	N	O	S	0	0	0
			1138	723	196	215	4			
1	E	150	Total	C	N	O	S	0	0	0
			1180	747	203	224	6			
1	F	151	Total	C	N	O	S	0	0	0
			1190	753	206	225	6			
1	G	143	Total	C	N	O	S	0	0	0
			1132	718	195	214	5			
1	H	142	Total	C	N	O	S	0	0	0
			1116	711	187	213	5			
1	I	135	Total	C	N	O	S	0	0	0
			1084	691	186	203	4			
1	J	140	Total	C	N	O	S	0	0	0
			1091	697	180	208	6			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	HIS	-	expression tag	UNP Q64339
A	76	SER	CYS	engineered mutation	UNP Q64339
B	0	HIS	-	expression tag	UNP Q64339
B	76	SER	CYS	engineered mutation	UNP Q64339
C	0	HIS	-	expression tag	UNP Q64339
C	76	SER	CYS	engineered mutation	UNP Q64339
D	0	HIS	-	expression tag	UNP Q64339
D	76	SER	CYS	engineered mutation	UNP Q64339
E	0	HIS	-	expression tag	UNP Q64339

*Continued on next page...*

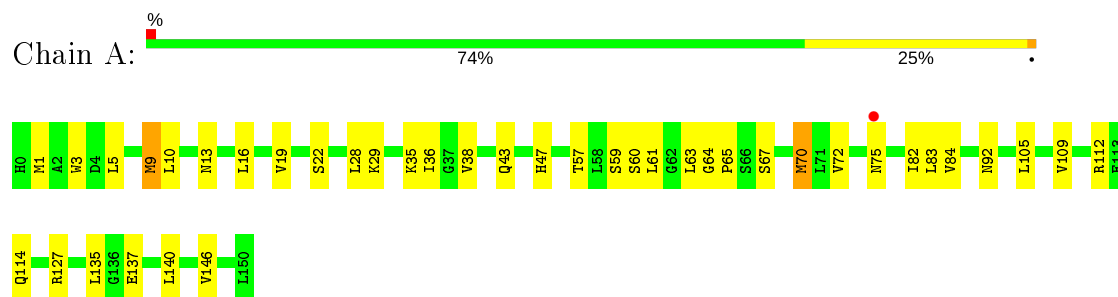
*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
E	76	SER	CYS	engineered mutation	UNP Q64339
F	0	HIS	-	expression tag	UNP Q64339
F	76	SER	CYS	engineered mutation	UNP Q64339
G	0	HIS	-	expression tag	UNP Q64339
G	76	SER	CYS	engineered mutation	UNP Q64339
H	0	HIS	-	expression tag	UNP Q64339
H	76	SER	CYS	engineered mutation	UNP Q64339
I	0	HIS	-	expression tag	UNP Q64339
I	76	SER	CYS	engineered mutation	UNP Q64339
J	0	HIS	-	expression tag	UNP Q64339
J	76	SER	CYS	engineered mutation	UNP Q64339

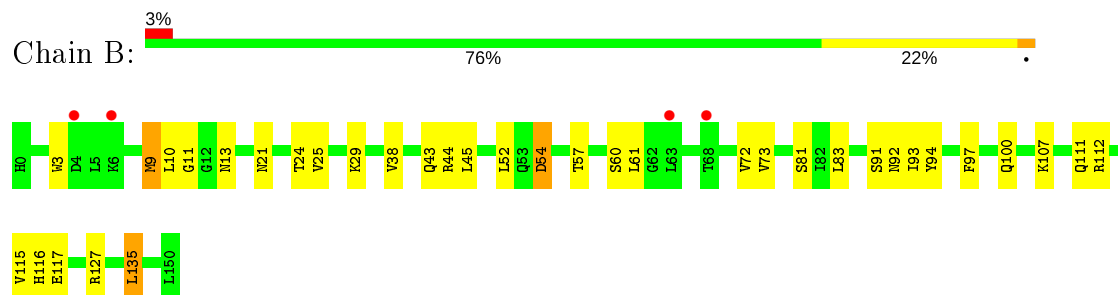
### 3 Residue-property plots [i](#)

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.

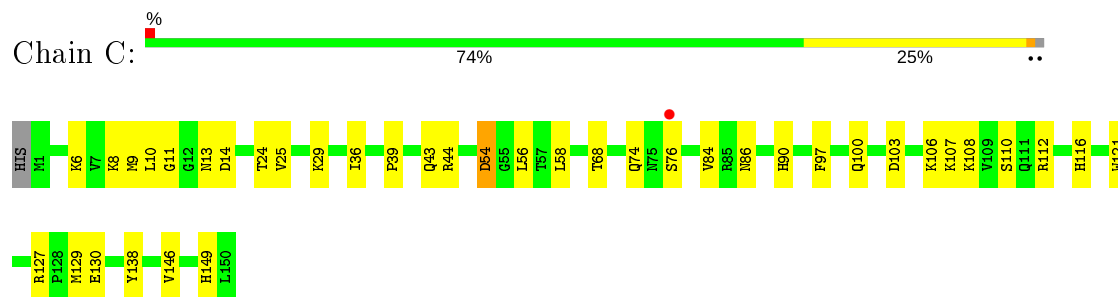
#### • Molecule 1: Ubiquitin-like protein ISG15



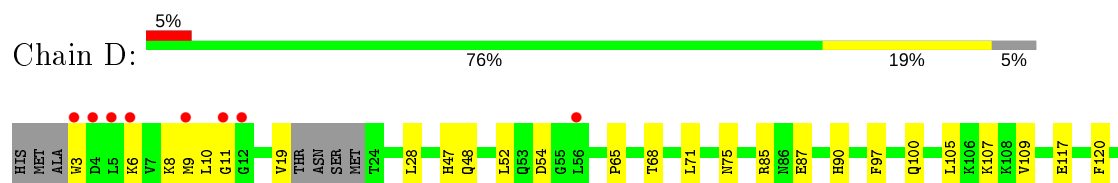
#### • Molecule 1: Ubiquitin-like protein ISG15

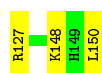


#### • Molecule 1: Ubiquitin-like protein ISG15

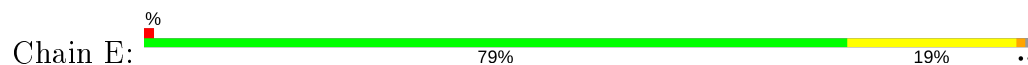


#### • Molecule 1: Ubiquitin-like protein ISG15

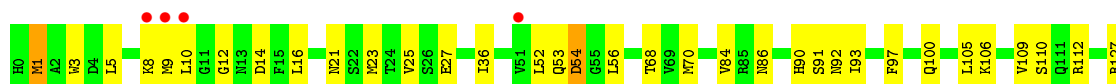




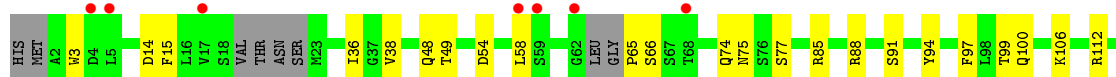
- Molecule 1: Ubiquitin-like protein ISG15



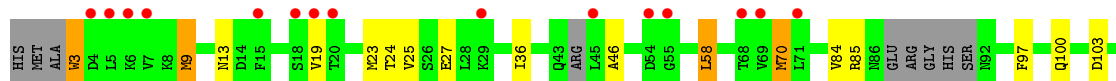
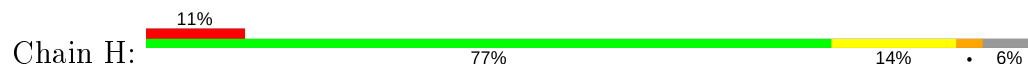
- Molecule 1: Ubiquitin-like protein ISG15



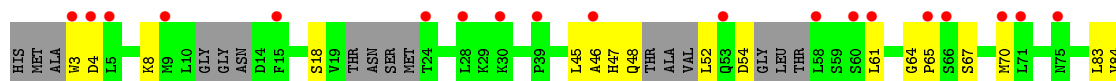
- Molecule 1: Ubiquitin-like protein ISG15

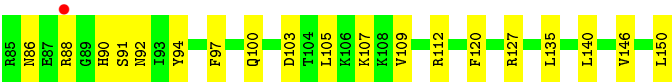


- Molecule 1: Ubiquitin-like protein ISG15

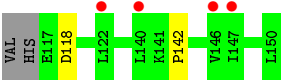
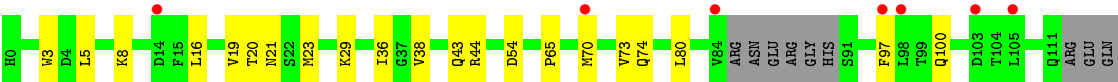
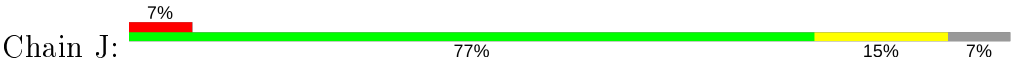


- Molecule 1: Ubiquitin-like protein ISG15





● Molecule 1: Ubiquitin-like protein ISG15





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	85.76 Å 60.16 Å 172.66 Å 90.00° 93.12° 90.00°	Depositor
Resolution (Å)	42.18 – 3.24 48.97 – 3.24	Depositor EDS
% Data completeness (in resolution range)	98.3 (42.18-3.24) 98.4 (48.97-3.24)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.75 (at 3.25 Å)	Xtriage
Refinement program	PHENIX dev_2420	Depositor
R, $R_{free}$	0.256 , 0.309 0.256 , 0.310	Depositor DCC
$R_{free}$ test set	1396 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	86.3	Xtriage
Anisotropy	0.661	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.24 , 33.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	11491	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	115.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.40% 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	0.25	0/1210	0.45	0/1632
1	B	0.25	0/1210	0.47	0/1632
1	C	0.25	0/1199	0.45	0/1617
1	D	0.25	0/1156	0.46	0/1558
1	E	0.25	0/1199	0.48	0/1617
1	F	0.24	0/1210	0.44	0/1632
1	G	0.24	0/1149	0.43	0/1545
1	H	0.24	0/1132	0.43	0/1526
1	I	0.24	0/1099	0.44	0/1475
1	J	0.25	0/1107	0.45	0/1492
All	All	0.24	0/11671	0.45	0/15726

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1190	0	1216	25	0
1	B	1190	0	1216	24	0
1	C	1180	0	1209	22	0
1	D	1138	0	1164	14	0
1	E	1180	0	1209	20	0
1	F	1190	0	1216	31	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	1132	0	1155	12	0
1	H	1116	0	1143	17	0
1	I	1084	0	1107	21	0
1	J	1091	0	1123	15	0
All	All	11491	0	11758	188	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 8.

All (188) 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:F:10:LEU:CD1	1:F:70:MET:CE	2.55	0.85
1:I:45:LEU:HB3	1:I:52:LEU:HD23	1.63	0.80
1:F:84:VAL:O	1:F:91:SER:HA	1.83	0.78
1:F:10:LEU:HD12	1:F:70:MET:HE3	1.68	0.76
1:F:10:LEU:CD1	1:F:70:MET:HE3	2.16	0.75
1:F:10:LEU:HD11	1:F:70:MET:HE2	1.68	0.75
1:A:9:MET:SD	1:A:13:ASN:ND2	2.62	0.73
1:D:6:LYS:NZ	1:D:65:PRO:O	2.24	0.71
1:A:114:GLN:OE1	1:C:13:ASN:ND2	2.25	0.70
1:I:46:ALA:O	1:I:70:MET:HB2	1.91	0.69
1:F:10:LEU:HD12	1:F:70:MET:CE	2.22	0.68
1:F:10:LEU:CD1	1:F:70:MET:HE2	2.23	0.68
1:J:5:LEU:O	1:J:16:LEU:HA	1.93	0.68
1:J:44:ARG:NH1	1:J:74:GLN:OE1	2.28	0.66
1:E:74:GLN:HE21	1:E:77:SER:HA	1.62	0.65
1:F:5:LEU:O	1:F:16:LEU:HA	1.98	0.64
1:I:52:LEU:HD12	1:I:61:LEU:HD22	1.79	0.64
1:D:8:LYS:HE3	1:D:68:THR:HG21	1.78	0.64
1:E:56:LEU:HD11	1:E:61:LEU:HD21	1.79	0.64
1:H:9:MET:HB3	1:H:13:ASN:HB2	1.80	0.63
1:I:8:LYS:HB3	1:I:70:MET:CE	2.30	0.62
1:I:4:ASP:HA	1:I:18:SER:HA	1.80	0.62
1:H:70:MET:N	1:H:70:MET:SD	2.67	0.61
1:A:70:MET:SD	1:A:70:MET:N	2.74	0.61
1:B:52:LEU:HD12	1:B:61:LEU:HD13	1.82	0.61
1:I:83:LEU:HA	1:I:92:ASN:O	2.01	0.60
1:B:115:VAL:HG12	1:B:116:HIS:H	1.66	0.60
1:E:57:THR:HG22	1:E:59:SER:H	1.67	0.60
1:F:36:ILE:HG23	1:G:112:ARG:HD2	1.84	0.59

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:92:ASN:HB3	1:F:112:ARG:HH21	1.67	0.58
1:C:103:ASP:OD2	1:C:107:LYS:NZ	2.32	0.58
1:A:5:LEU:O	1:A:16:LEU:HA	2.04	0.57
1:B:9:MET:HB3	1:B:13:ASN:HB2	1.87	0.57
1:H:19:VAL:HG11	1:H:58:LEU:HD11	1.85	0.57
1:I:47:HIS:N	1:I:48:GLN:HA	2.20	0.56
1:D:47:HIS:HB3	1:D:52:LEU:HD21	1.86	0.56
1:D:97:PHE:HB2	1:D:100:GLN:HG3	1.87	0.56
1:F:93:ILE:O	1:F:112:ARG:NH2	2.39	0.55
1:F:53:GLN:HB3	1:F:56:LEU:HG	1.88	0.55
1:C:8:LYS:HG3	1:C:14:ASP:HB3	1.88	0.55
1:C:6:LYS:HD3	1:C:68:THR:HG22	1.88	0.54
1:H:103:ASP:OD2	1:H:107:LYS:NZ	2.34	0.54
1:B:45:LEU:HB3	1:B:52:LEU:HD23	1.90	0.54
1:C:6:LYS:NZ	1:C:14:ASP:OD2	2.40	0.54
1:A:35:LYS:NZ	1:B:111:GLN:OE1	2.40	0.54
1:C:97:PHE:HB2	1:C:100:GLN:HG3	1.90	0.53
1:D:107:LYS:HG2	1:D:117:GLU:OE2	2.09	0.53
1:F:23:MET:HG3	1:F:27:GLU:HB2	1.91	0.53
1:I:84:VAL:HA	1:I:146:VAL:O	2.08	0.53
1:C:74:GLN:HG3	1:C:76:SER:O	2.08	0.53
1:G:85:ARG:HG2	1:G:91:SER:HB2	1.89	0.53
1:H:3:TRP:N	1:H:19:VAL:O	2.42	0.53
1:F:106:LYS:O	1:F:110:SER:HB2	2.09	0.52
1:E:86:ASN:OD1	1:E:87:GLU:N	2.42	0.52
1:I:135:LEU:HB3	1:I:140:LEU:HD22	1.92	0.52
1:G:97:PHE:HB2	1:G:100:GLN:HG3	1.92	0.52
1:A:57:THR:HG22	1:A:59:SER:H	1.74	0.51
1:H:9:MET:N	1:H:13:ASN:O	2.42	0.51
1:E:97:PHE:HB2	1:E:100:GLN:HG3	1.92	0.51
1:F:86:ASN:OD1	1:F:90:HIS:N	2.42	0.51
1:H:24:THR:OG1	1:H:25:VAL:N	2.43	0.51
1:I:64:GLY:H	1:I:67:SER:HB2	1.76	0.51
1:E:56:LEU:CD1	1:E:61:LEU:HD21	2.41	0.51
1:F:8:LYS:HG2	1:F:14:ASP:HB3	1.92	0.50
1:I:84:VAL:O	1:I:91:SER:HA	2.11	0.50
1:J:29:LYS:HD2	1:J:43:GLN:HB2	1.93	0.50
1:E:44:ARG:HB2	1:E:74:GLN:OE1	2.12	0.50
1:A:82:ILE:HD12	1:A:146:VAL:HG21	1.92	0.50
1:F:53:GLN:OE1	1:F:54:ASP:N	2.41	0.50
1:A:84:VAL:HA	1:A:146:VAL:O	2.12	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:84:VAL:HG13	1:H:146:VAL:HG23	1.92	0.50
1:I:94:TYR:CZ	1:I:112:ARG:HD3	2.47	0.50
1:B:44:ARG:HB3	1:B:72:VAL:O	2.11	0.50
1:H:84:VAL:HA	1:H:146:VAL:O	2.12	0.50
1:J:80:LEU:HD12	1:J:142:PRO:HA	1.94	0.50
1:J:20:THR:HG22	1:J:21:ASN:H	1.76	0.49
1:J:8:LYS:HD2	1:J:70:MET:HE1	1.93	0.49
1:G:106:LYS:HE3	1:G:117:GLU:HG2	1.95	0.49
1:A:64:GLY:H	1:A:67:SER:HB2	1.77	0.49
1:F:97:PHE:HB2	1:F:100:GLN:HG3	1.94	0.49
1:F:92:ASN:HB3	1:F:112:ARG:NH2	2.28	0.49
1:G:74:GLN:HG3	1:G:77:SER:HA	1.95	0.49
1:B:9:MET:N	1:B:13:ASN:O	2.45	0.49
1:C:29:LYS:HD2	1:C:43:GLN:HB2	1.94	0.49
1:F:86:ASN:HD21	1:F:90:HIS:HB2	1.78	0.48
1:A:57:THR:O	1:A:60:SER:OG	2.26	0.48
1:A:1:MET:SD	1:G:99:THR:OG1	2.71	0.48
1:C:58:LEU:HD12	1:C:58:LEU:H	1.79	0.48
1:C:112:ARG:HD2	1:E:36:ILE:HG23	1.96	0.48
1:A:19:VAL:HG11	1:A:28:LEU:HD23	1.94	0.48
1:B:83:LEU:HD22	1:B:91:SER:HB3	1.96	0.48
1:G:36:ILE:HG22	1:G:38:VAL:HG12	1.96	0.48
1:I:3:TRP:HE3	1:I:65:PRO:HG3	1.78	0.48
1:B:29:LYS:HD2	1:B:43:GLN:HB2	1.95	0.47
1:F:3:TRP:NE1	1:F:21:ASN:OD1	2.47	0.47
1:B:24:THR:OG1	1:B:25:VAL:N	2.47	0.47
1:H:23:MET:HG3	1:H:27:GLU:HB2	1.94	0.47
1:F:10:LEU:HD11	1:F:70:MET:CE	2.30	0.47
1:A:112:ARG:HD2	1:C:36:ILE:HG23	1.95	0.47
1:G:65:PRO:HA	1:G:66:SER:HA	1.60	0.47
1:I:103:ASP:OD2	1:I:107:LYS:NZ	2.35	0.47
1:D:10:LEU:HA	1:D:11:GLY:C	2.34	0.47
1:E:3:TRP:CE3	1:E:65:PRO:HG3	2.50	0.47
1:E:107:LYS:HG2	1:E:117:GLU:OE2	2.15	0.47
1:H:97:PHE:HB2	1:H:100:GLN:HG3	1.97	0.47
1:F:142:PRO:HG2	1:H:130:GLU:HG3	1.97	0.47
1:F:25:VAL:HG11	1:F:52:LEU:HB3	1.97	0.47
1:I:97:PHE:HB2	1:I:100:GLN:HG3	1.97	0.47
1:A:135:LEU:HB3	1:A:140:LEU:HD22	1.97	0.46
1:C:86:ASN:N	1:C:90:HIS:O	2.47	0.46
1:B:97:PHE:HB2	1:B:100:GLN:HG3	1.97	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:8:LYS:HB3	1:I:70:MET:HE1	1.96	0.46
1:A:61:LEU:HD23	1:A:63:LEU:HD22	1.98	0.46
1:F:106:LYS:O	1:F:110:SER:CB	2.63	0.46
1:F:8:LYS:HE3	1:F:68:THR:HG21	1.98	0.46
1:I:86:ASN:ND2	1:I:90:HIS:O	2.48	0.46
1:C:121:TRP:O	1:C:149:HIS:HB2	2.17	0.46
1:D:85:ARG:O	1:D:148:LYS:HB3	2.16	0.46
1:H:108:LYS:HB3	1:J:36:ILE:O	2.15	0.45
1:A:29:LYS:HD2	1:A:43:GLN:HB2	1.98	0.45
1:B:25:VAL:HB	1:B:54:ASP:HA	1.98	0.45
1:E:26:SER:OG	1:E:54:ASP:HB3	2.16	0.45
1:J:19:VAL:HG23	1:J:23:MET:SD	2.56	0.45
1:C:25:VAL:HB	1:C:54:ASP:HA	1.98	0.45
1:F:1:MET:SD	1:F:1:MET:N	2.90	0.45
1:E:29:LYS:HD2	1:E:43:GLN:HB2	1.99	0.45
1:E:25:VAL:HB	1:E:54:ASP:HA	1.99	0.45
1:H:112:ARG:HD2	1:J:36:ILE:HG23	1.98	0.45
1:J:8:LYS:HB3	1:J:70:MET:SD	2.56	0.45
1:C:39:PRO:O	1:C:43:GLN:HG3	2.17	0.45
1:J:97:PHE:HB2	1:J:100:GLN:HG3	1.99	0.45
1:C:129:MET:HA	1:C:138:TYR:CE2	2.51	0.45
1:B:29:LYS:O	1:B:43:GLN:NE2	2.43	0.45
1:E:8:LYS:HG3	1:E:14:ASP:HB2	1.98	0.44
1:I:3:TRP:CE3	1:I:65:PRO:HG3	2.51	0.44
1:A:3:TRP:HZ3	1:A:5:LEU:HD13	1.82	0.44
1:A:47:HIS:NE2	1:A:67:SER:OG	2.50	0.44
1:B:10:LEU:HD23	1:B:11:GLY:HA2	1.99	0.44
1:D:105:LEU:O	1:D:109:VAL:HG12	2.18	0.43
1:A:3:TRP:CE3	1:A:65:PRO:HG3	2.53	0.43
1:B:10:LEU:HA	1:B:11:GLY:HA2	1.57	0.43
1:D:120:PHE:HA	1:D:150:LEU:HB3	1.99	0.43
1:D:9:MET:HG3	1:D:71:LEU:HD23	2.00	0.43
1:F:9:MET:HG3	1:F:12:GLY:HA3	1.99	0.43
1:E:77:SER:HB2	1:E:99:THR:HG23	2.00	0.43
1:J:3:TRP:O	1:J:19:VAL:N	2.47	0.43
1:A:137:GLU:OE1	1:B:81:SER:HB3	2.19	0.43
1:I:120:PHE:HA	1:I:150:LEU:HB3	2.00	0.43
1:B:94:TYR:CZ	1:B:112:ARG:HD3	2.54	0.43
1:H:46:ALA:HB3	1:H:70:MET:SD	2.59	0.43
1:E:74:GLN:NE2	1:E:77:SER:HA	2.31	0.42
1:D:47:HIS:CE1	1:D:48:GLN:HG2	2.54	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3:TRP:CE3	1:D:65:PRO:HG3	2.54	0.42
1:E:14:ASP:OD1	1:E:15:PHE:N	2.53	0.42
1:B:83:LEU:HA	1:B:92:ASN:O	2.19	0.42
1:C:24:THR:HA	1:C:56:LEU:O	2.20	0.42
1:G:58:LEU:HD12	1:G:58:LEU:H	1.85	0.42
1:A:36:ILE:HG22	1:A:38:VAL:HG12	2.01	0.42
1:B:38:VAL:HG21	1:B:73:VAL:HG12	2.01	0.42
1:A:83:LEU:HA	1:A:92:ASN:O	2.19	0.42
1:C:106:LYS:O	1:C:110:SER:HB2	2.20	0.42
1:C:130:GLU:N	1:C:138:TYR:OH	2.51	0.41
1:F:105:LEU:O	1:F:109:VAL:HG12	2.20	0.41
1:G:14:ASP:OD1	1:G:15:PHE:N	2.53	0.41
1:B:93:ILE:O	1:B:112:ARG:NH1	2.42	0.41
1:G:48:GLN:O	1:G:49:THR:OG1	2.36	0.41
1:B:57:THR:HG23	1:B:60:SER:H	1.84	0.41
1:E:106:LYS:O	1:E:110:SER:HB2	2.19	0.41
1:C:108:LYS:HE2	1:E:34:GLN:O	2.21	0.41
1:F:112:ARG:HD3	1:H:36:ILE:HG23	2.02	0.41
1:J:3:TRP:CE3	1:J:65:PRO:HG3	2.56	0.41
1:E:77:SER:O	1:E:97:PHE:HD2	2.02	0.41
1:D:19:VAL:HG11	1:D:28:LEU:HD23	2.01	0.41
1:D:87:GLU:CD	1:D:87:GLU:H	2.24	0.41
1:B:107:LYS:HG2	1:B:117:GLU:OE2	2.19	0.41
1:F:142:PRO:HB3	1:H:133:GLU:OE1	2.21	0.41
1:I:64:GLY:H	1:I:67:SER:CB	2.34	0.41
1:A:105:LEU:O	1:A:109:VAL:HG12	2.21	0.40
1:B:100:GLN:O	1:B:135:LEU:HD12	2.21	0.40
1:C:10:LEU:HD23	1:C:11:GLY:N	2.35	0.40
1:G:94:TYR:CZ	1:G:112:ARG:HD3	2.57	0.40
1:A:22:SER:HA	1:A:57:THR:HG23	2.03	0.40
1:B:3:TRP:HE1	1:B:21:ASN:HB2	1.87	0.40
1:I:105:LEU:O	1:I:109:VAL:HG12	2.22	0.40
1:A:10:LEU:HD12	1:A:72:VAL:HG22	2.04	0.40
1:C:84:VAL:HA	1:C:146:VAL:O	2.22	0.40
1:J:118:ASP:OD1	1:J:118:ASP:N	2.55	0.40
1:J:38:VAL:HG21	1:J:73:VAL:HG12	2.03	0.40

There are no symmetry-related clashes.

## 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	149/151 (99%)	147 (99%)	2 (1%)	0	100	100
1	B	149/151 (99%)	149 (100%)	0	0	100	100
1	C	148/151 (98%)	146 (99%)	2 (1%)	0	100	100
1	D	140/151 (93%)	137 (98%)	3 (2%)	0	100	100
1	E	148/151 (98%)	148 (100%)	0	0	100	100
1	F	149/151 (99%)	145 (97%)	4 (3%)	0	100	100
1	G	137/151 (91%)	137 (100%)	0	0	100	100
1	H	136/151 (90%)	135 (99%)	1 (1%)	0	100	100
1	I	125/151 (83%)	125 (100%)	0	0	100	100
1	J	134/151 (89%)	133 (99%)	1 (1%)	0	100	100
All	All	1415/1510 (94%)	1402 (99%)	13 (1%)	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	A	136/136 (100%)	132 (97%)	4 (3%)	42	71
1	B	136/136 (100%)	132 (97%)	4 (3%)	42	71
1	C	135/136 (99%)	130 (96%)	5 (4%)	34	66
1	D	130/136 (96%)	126 (97%)	4 (3%)	40	70

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	135/136 (99%)	130 (96%)	5 (4%)	34	66
1	F	136/136 (100%)	132 (97%)	4 (3%)	42	71
1	G	129/136 (95%)	124 (96%)	5 (4%)	32	65
1	H	129/136 (95%)	122 (95%)	7 (5%)	22	55
1	I	125/136 (92%)	122 (98%)	3 (2%)	49	75
1	J	126/136 (93%)	125 (99%)	1 (1%)	81	91
All	All	1317/1360 (97%)	1275 (97%)	42 (3%)	39	69

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	MET
1	A	70	MET
1	A	75	ASN
1	A	127	ARG
1	B	9	MET
1	B	54	ASP
1	B	127	ARG
1	B	135	LEU
1	C	9	MET
1	C	44	ARG
1	C	54	ASP
1	C	116	HIS
1	C	127	ARG
1	D	54	ASP
1	D	75	ASN
1	D	90	HIS
1	D	127	ARG
1	E	1	MET
1	E	54	ASP
1	E	56	LEU
1	E	75	ASN
1	E	127	ARG
1	F	1	MET
1	F	54	ASP
1	F	127	ARG
1	F	150	LEU
1	G	3	TRP
1	G	54	ASP
1	G	75	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	G	88	ARG
1	G	127	ARG
1	H	3	TRP
1	H	9	MET
1	H	58	LEU
1	H	70	MET
1	H	85	ARG
1	H	116	HIS
1	H	127	ARG
1	I	54	ASP
1	I	88	ARG
1	I	127	ARG
1	J	54	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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

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	A	151/151 (100%)	-0.13	1 (0%) 87 83	53, 84, 126, 144	0
1	B	151/151 (100%)	-0.05	4 (2%) 56 44	54, 88, 139, 161	0
1	C	150/151 (99%)	-0.20	1 (0%) 87 83	56, 86, 127, 152	0
1	D	144/151 (95%)	0.10	8 (5%) 24 15	56, 96, 182, 193	0
1	E	150/151 (99%)	-0.08	2 (1%) 77 68	57, 102, 150, 172	0
1	F	151/151 (100%)	-0.06	4 (2%) 56 44	78, 117, 156, 180	0
1	G	143/151 (94%)	0.34	7 (4%) 29 19	74, 123, 195, 225	0
1	H	142/151 (94%)	0.57	16 (11%) 5 4	90, 149, 196, 206	0
1	I	135/151 (89%)	0.81	20 (14%) 2 2	81, 126, 213, 241	0
1	J	140/151 (92%)	0.34	11 (7%) 12 8	102, 148, 178, 228	0
All	All	1457/1510 (96%)	0.15	74 (5%) 28 18	53, 112, 186, 241	0

All (74) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	4	ASP	7.2
1	H	54	ASP	6.7
1	H	20	THR	6.6
1	I	58	LEU	5.8
1	I	3	TRP	5.6
1	G	4	ASP	5.5
1	I	9	MET	5.2
1	H	19	VAL	4.9
1	G	5	LEU	4.7
1	H	5	LEU	4.2
1	D	12	GLY	4.2
1	F	9	MET	4.1
1	D	11	GLY	3.9

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	I	60	SER	3.8
1	J	146	VAL	3.6
1	I	28	LEU	3.5
1	H	69	VAL	3.5
1	H	6	LYS	3.5
1	H	45	LEU	3.4
1	I	46	ALA	3.2
1	J	84	VAL	3.1
1	H	18	SER	3.1
1	G	62	GLY	3.1
1	H	7	VAL	3.1
1	I	66	SER	3.0
1	F	51	VAL	3.0
1	B	4	ASP	3.0
1	D	56	LEU	2.9
1	B	68	THR	2.9
1	I	5	LEU	2.9
1	I	24	THR	2.9
1	H	55	GLY	2.9
1	I	75	ASN	2.8
1	H	4	ASP	2.8
1	G	68	THR	2.8
1	H	71	LEU	2.8
1	I	39	PRO	2.8
1	J	105	LEU	2.7
1	H	29	LYS	2.7
1	I	88	ARG	2.7
1	D	6	LYS	2.6
1	G	59	SER	2.6
1	I	71	LEU	2.6
1	F	8	LYS	2.5
1	E	10	LEU	2.5
1	H	15	PHE	2.5
1	I	61	LEU	2.5
1	G	17	VAL	2.4
1	D	5	LEU	2.4
1	D	4	ASP	2.4
1	G	58	LEU	2.4
1	B	6	LYS	2.4
1	D	3	TRP	2.3
1	I	70	MET	2.3
1	I	53	GLN	2.3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	I	65	PRO	2.3
1	J	97	PHE	2.3
1	J	103	ASP	2.3
1	B	63	LEU	2.3
1	E	140	LEU	2.3
1	J	70	MET	2.2
1	H	68	THR	2.2
1	I	30	LYS	2.2
1	J	14	ASP	2.2
1	J	147	ILE	2.2
1	J	122	LEU	2.2
1	H	146	VAL	2.2
1	A	75	ASN	2.2
1	J	98	LEU	2.1
1	I	15	PHE	2.1
1	J	140	LEU	2.1
1	F	10	LEU	2.1
1	C	76	SER	2.0
1	D	9	MET	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.