



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 02:07 PM GMT

PDB ID : 3VON  
Title : Crystalstructure of the ubiquitin protease  
Authors : Sato, Y.; Fukai, S.  
Deposited on : 2012-01-30  
Resolution : 3.15 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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  
<http://wwpdb.org/validation/2016/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  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

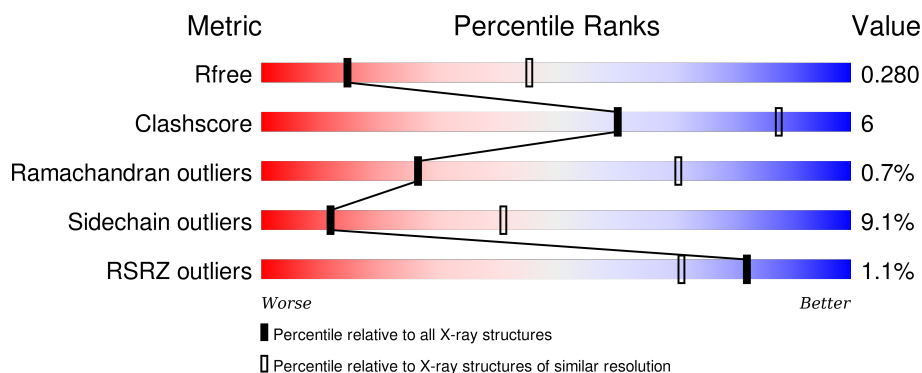
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.15 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))
$R_{free}$	91344	1112 (3.20-3.12)
Clashscore	102246	1249 (3.20-3.12)
Ramachandran outliers	100387	1222 (3.20-3.12)
Sidechain outliers	100360	1221 (3.20-3.12)
RSRZ outliers	91569	1117 (3.20-3.12)

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. 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	228	<div> <div></div> <div>77% 13% • 8%</div> </div>
1	H	228	<div> <div>9%</div> <div>78% 14% • 6%</div> </div>
1	O	228	<div> <div></div> <div>77% 16% • 5%</div> </div>
1	V	228	<div> <div>%</div> <div>81% 12% • 6%</div> </div>
1	c	228	<div> <div>4%</div> <div>87% 8% 5%</div> </div>









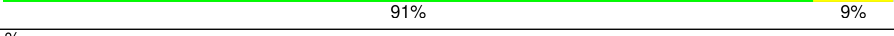

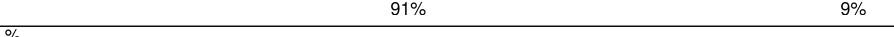

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Mol	Chain	Length	Quality of chain
1	j	228	<div> <div>9%</div> <div>83%</div> <div>9%</div> <div>8%</div> </div>
2	B	138	<div> <div>%</div> <div>86%</div> <div>14%</div> </div>
2	D	138	<div> <div>75%</div> <div>22%</div> <div>..</div> </div>
2	F	138	<div> <div>71%</div> <div>24%</div> <div>5%</div> </div>
2	I	138	<div> <div>70%</div> <div>24%</div> <div>6%</div> <div>.</div> </div>
2	K	138	<div> <div>%</div> <div>70%</div> <div>28%</div> <div>.</div> </div>
2	M	138	<div> <div>71%</div> <div>27%</div> <div>.</div> </div>
2	P	138	<div> <div>%</div> <div>86%</div> <div>13%</div> <div>.</div> </div>
2	R	138	<div> <div>88%</div> <div>11%</div> <div>..</div> </div>
2	T	138	<div> <div>83%</div> <div>14%</div> <div>.</div> </div>
2	W	138	<div> <div>79%</div> <div>19%</div> <div>..</div> </div>
2	Y	138	<div> <div>86%</div> <div>10%</div> <div>..</div> </div>
2	a	138	<div> <div>%</div> <div>93%</div> <div>6%</div> <div>.</div> </div>
2	d	138	<div> <div>%</div> <div>93%</div> <div>7%</div> </div>
2	f	138	<div> <div>90%</div> <div>9%</div> <div>.</div> </div>
2	h	138	<div> <div>93%</div> <div>7%</div> </div>
2	k	138	<div> <div>91%</div> <div>9%</div> </div>
2	m	138	<div> <div>96%</div> <div>..</div> </div>
2	o	138	<div> <div>93%</div> <div>7%</div> </div>
3	C	148	<div> <div>%</div> <div>68%</div> <div>23%</div> <div>7%</div> <div>..</div> </div>
3	E	148	<div> <div>69%</div> <div>25%</div> <div>5%</div> <div>..</div> </div>
3	G	148	<div> <div>61%</div> <div>30%</div> <div>7%</div> <div>..</div> </div>
3	J	148	<div> <div>74%</div> <div>22%</div> <div>..</div> </div>
3	L	148	<div> <div>%</div> <div>70%</div> <div>26%</div> <div>..</div> </div>
3	N	148	<div> <div>%</div> <div>66%</div> <div>29%</div> <div>5%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
3	Q	148	 80% 16% . .
3	S	148	 76% 21% .
3	U	148	 78% 18% . .
3	X	148	 74% 22% . .
3	Z	148	 81% 18% .
3	b	148	 91% 8% .
3	e	148	 88% 9% . .
3	g	148	 91% 9%
3	i	148	 91% 9%
3	l	148	 89% 9% . .
3	n	148	 91% 9% .
3	p	148	 90% 9% .

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 51450 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 thioesterase OTUB1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	210	Total	C	N	O	S	0	0	0
			1731	1111	284	330	6			
1	H	214	Total	C	N	O	S	0	0	0
			1767	1133	290	339	5			
1	O	216	Total	C	N	O	S	0	0	0
			1786	1148	292	340	6			
1	V	215	Total	C	N	O	S	0	0	0
			1777	1140	292	339	6			
1	c	217	Total	C	N	O	S	0	0	0
			1785	1144	293	342	6			
1	j	210	Total	C	N	O	S	0	0	0
			1730	1112	284	329	5			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	44	SER	-	EXPRESSION TAG	UNP Q96FW1
H	44	SER	-	EXPRESSION TAG	UNP Q96FW1
O	44	SER	-	EXPRESSION TAG	UNP Q96FW1
V	44	SER	-	EXPRESSION TAG	UNP Q96FW1
c	44	SER	-	EXPRESSION TAG	UNP Q96FW1
j	44	SER	-	EXPRESSION TAG	UNP Q96FW1

- Molecule 2 is a protein called Ubiquitin-conjugating enzyme E2 variant 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	138	Total	C	N	O	S	0	0	0
			1096	689	191	208	8			
2	D	137	Total	C	N	O	S	0	0	0
			1092	687	190	207	8			
2	F	138	Total	C	N	O	S	0	0	0
			1096	689	191	208	8			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	I	138	Total	C	N	O	S	0	0	0
			1096	689	191	208	8			
2	K	138	Total	C	N	O	S	0	0	0
			1096	689	191	208	8			
2	M	138	Total	C	N	O	S	0	0	0
			1096	689	191	208	8			
2	P	138	Total	C	N	O	S	0	0	0
			1096	689	191	208	8			
2	R	137	Total	C	N	O	S	0	0	0
			1092	687	190	207	8			
2	T	138	Total	C	N	O	S	0	0	0
			1096	689	191	208	8			
2	W	137	Total	C	N	O	S	0	0	0
			1092	687	190	207	8			
2	Y	137	Total	C	N	O	S	0	0	0
			1092	687	190	207	8			
2	a	138	Total	C	N	O	S	0	0	0
			1096	689	191	208	8			
2	d	138	Total	C	N	O	S	0	0	0
			1096	689	191	208	8			
2	f	137	Total	C	N	O	S	0	0	0
			1092	687	190	207	8			
2	h	138	Total	C	N	O	S	0	0	0
			1096	689	191	208	8			
2	k	138	Total	C	N	O	S	0	0	0
			1096	689	191	208	8			
2	m	137	Total	C	N	O	S	0	0	0
			1092	687	190	207	8			
2	o	138	Total	C	N	O	S	0	0	0
			1096	689	191	208	8			

- Molecule 3 is a protein called Ubiquitin-conjugating enzyme E2 N.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	147	Total	C	N	O	S	0	0	0
			1175	755	202	214	4			
3	E	147	Total	C	N	O	S	0	0	0
			1175	755	202	214	4			
3	G	147	Total	C	N	O	S	0	0	0
			1175	755	202	214	4			
3	J	147	Total	C	N	O	S	0	0	0
			1175	755	202	214	4			

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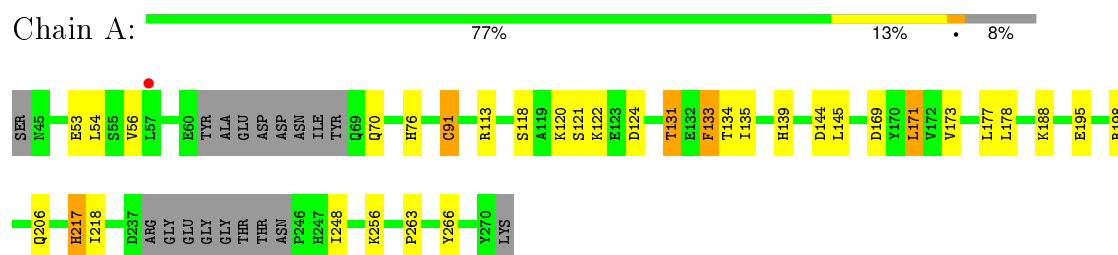
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	147	Total	C	N	O	S	0	0	0
			1175	755	202	214	4			
3	N	147	Total	C	N	O	S	0	0	0
			1175	755	202	214	4			
3	Q	147	Total	C	N	O	S	0	0	0
			1175	755	202	214	4			
3	S	148	Total	C	N	O	S	0	0	0
			1179	757	203	215	4			
3	U	147	Total	C	N	O	S	0	0	0
			1175	755	202	214	4			
3	X	147	Total	C	N	O	S	0	0	0
			1175	755	202	214	4			
3	Z	148	Total	C	N	O	S	0	0	0
			1179	757	203	215	4			
3	b	147	Total	C	N	O	S	0	0	0
			1175	755	202	214	4			
3	e	147	Total	C	N	O	S	0	0	0
			1175	755	202	214	4			
3	g	148	Total	C	N	O	S	0	0	0
			1179	757	203	215	4			
3	i	148	Total	C	N	O	S	0	0	0
			1179	757	203	215	4			
3	l	147	Total	C	N	O	S	0	0	0
			1175	755	202	214	4			
3	n	147	Total	C	N	O	S	0	0	0
			1175	755	202	214	4			
3	p	148	Total	C	N	O	S	0	0	0
			1179	757	203	215	4			

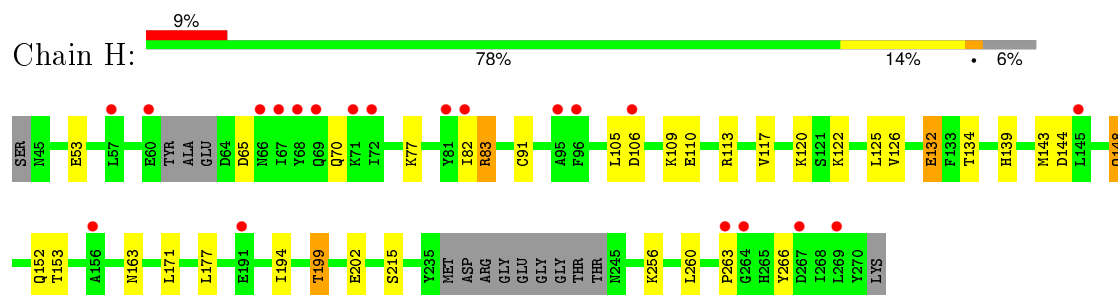
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

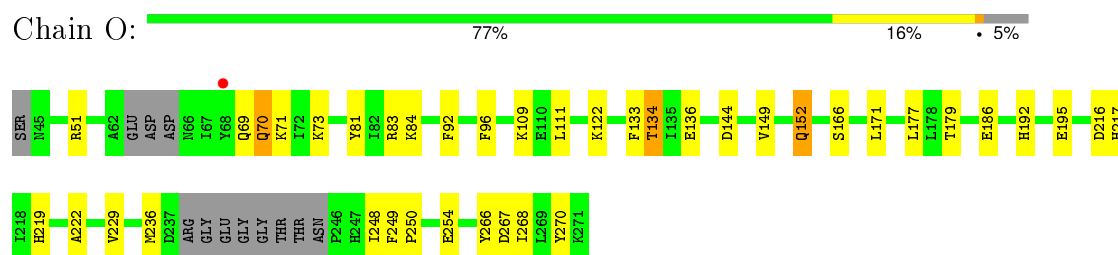
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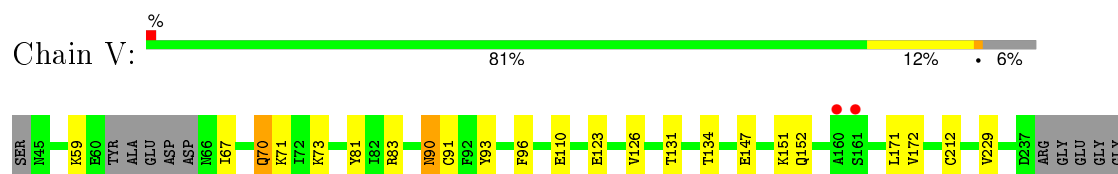
#### • Molecule 1: Ubiquitin thioesterase OTUB1



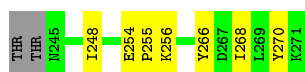
#### • Molecule 1: Ubiquitin thioesterase OTUB1



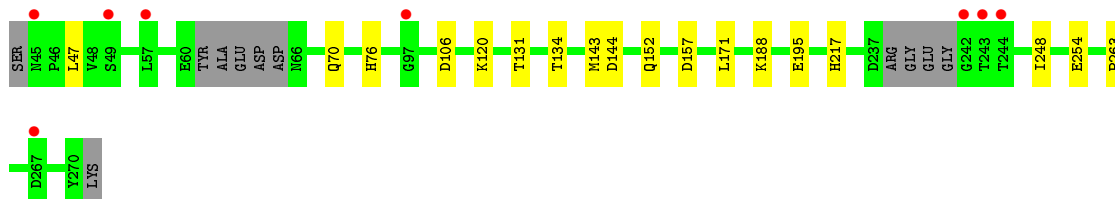
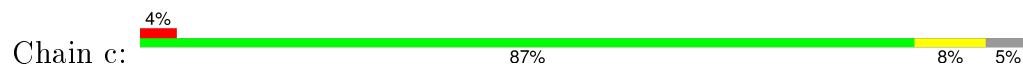
#### • Molecule 1: Ubiquitin thioesterase OTUB1



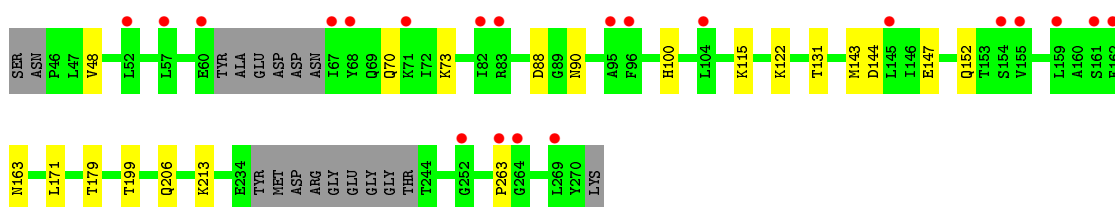
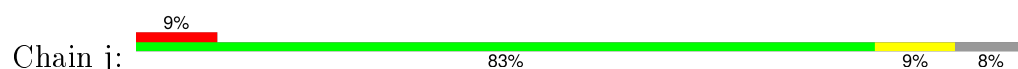




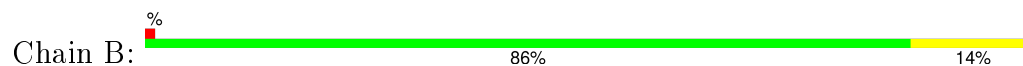
• Molecule 1: Ubiquitin thioesterase OTUB1



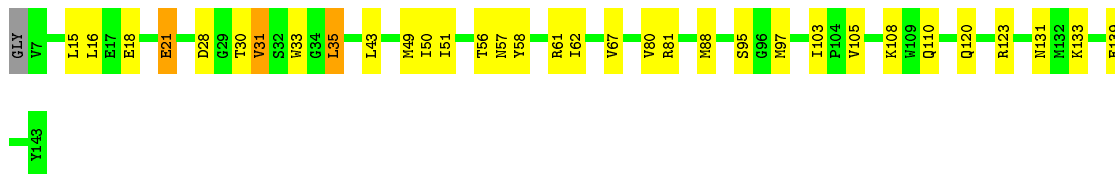
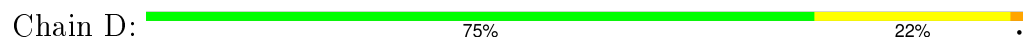
• Molecule 1: Ubiquitin thioesterase OTUB1



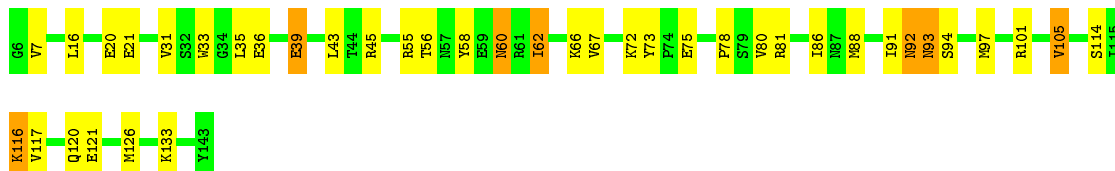
• Molecule 2: Ubiquitin-conjugating enzyme E2 variant 2



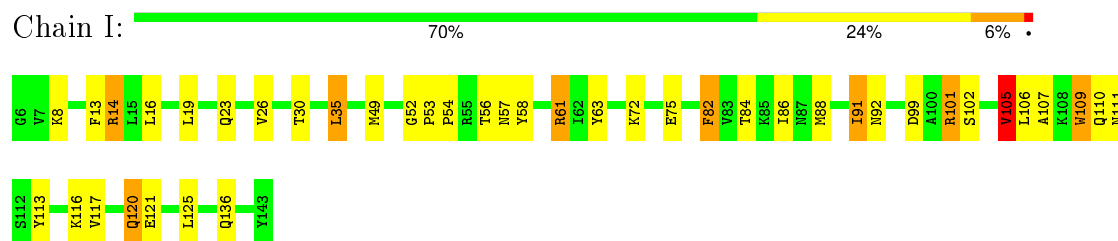
• Molecule 2: Ubiquitin-conjugating enzyme E2 variant 2



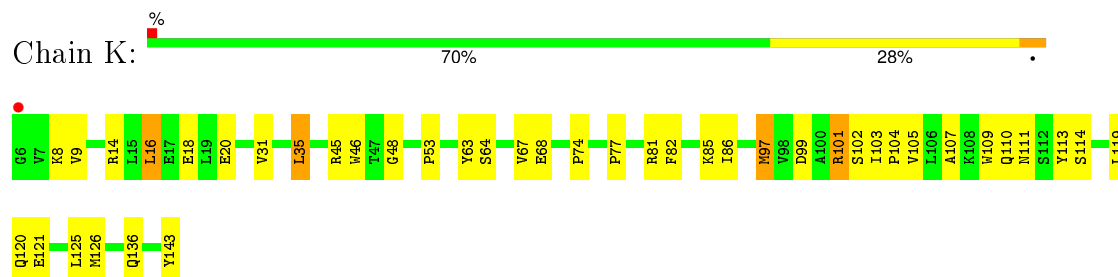
• Molecule 2: Ubiquitin-conjugating enzyme E2 variant 2



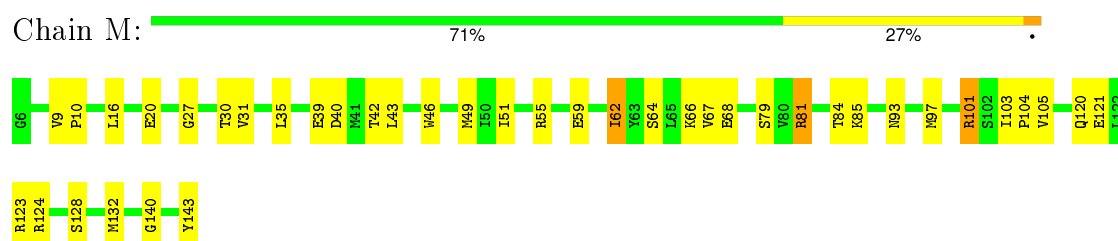
- Molecule 2: Ubiquitin-conjugating enzyme E2 variant 2



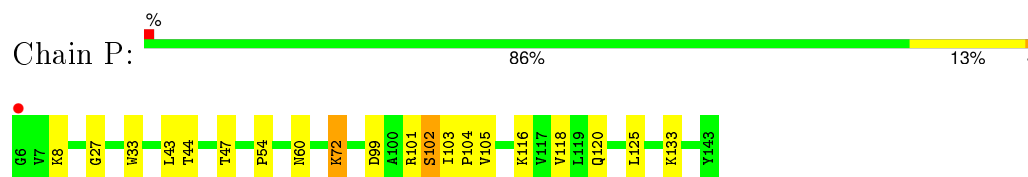
- Molecule 2: Ubiquitin-conjugating enzyme E2 variant 2



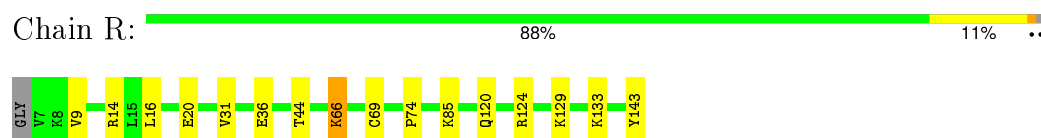
- Molecule 2: Ubiquitin-conjugating enzyme E2 variant 2



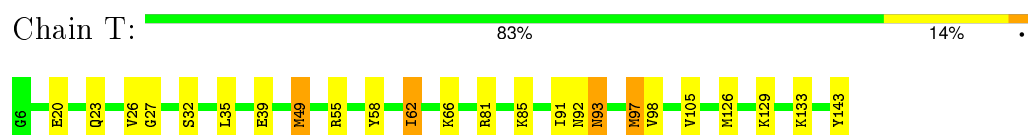
- Molecule 2: Ubiquitin-conjugating enzyme E2 variant 2




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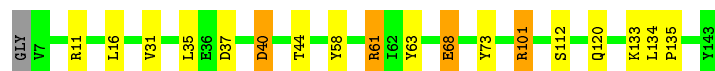
- Molecule 2: Ubiquitin-conjugating enzyme E2 variant 2

Chain W:  79% 19% ..

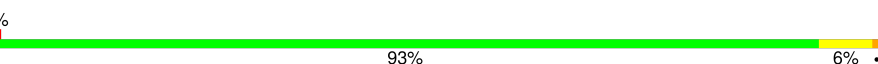


- Molecule 2: Ubiquitin-conjugating enzyme E2 variant 2

Chain Y:  86% 10% ..

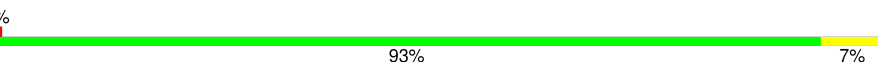


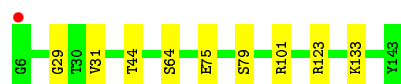
- Molecule 2: Ubiquitin-conjugating enzyme E2 variant 2

Chain a:  93% 6% .



- Molecule 2: Ubiquitin-conjugating enzyme E2 variant 2

Chain d:  93% 7%



- Molecule 2: Ubiquitin-conjugating enzyme E2 variant 2

Chain f:  90% 9% .




- Molecule 2: Ubiquitin-conjugating enzyme E2 variant 2

Chain h:  93% 7%



- Molecule 2: Ubiquitin-conjugating enzyme E2 variant 2

Chain k:  91% 9%



- Molecule 2: Ubiquitin-conjugating enzyme E2 variant 2

Chain m:  96% ..



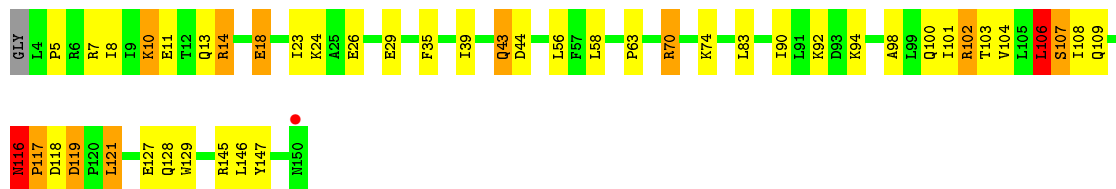
- Molecule 2: Ubiquitin-conjugating enzyme E2 variant 2

Chain o:  93% 7%



- Molecule 3: Ubiquitin-conjugating enzyme E2 N

Chain C:  68% 23% 7% ..



- Molecule 3: Ubiquitin-conjugating enzyme E2 N

Chain E:  69% 25% 5% ..



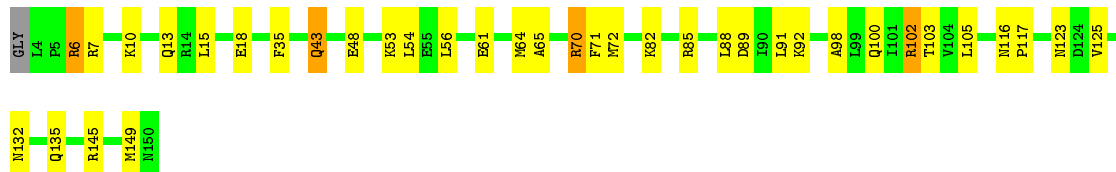
- Molecule 3: Ubiquitin-conjugating enzyme E2 N

Chain G:  61% 30% 7% ..

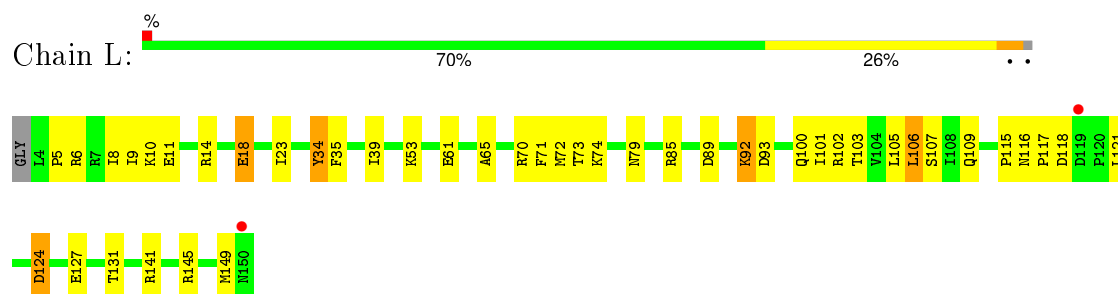


- Molecule 3: Ubiquitin-conjugating enzyme E2 N

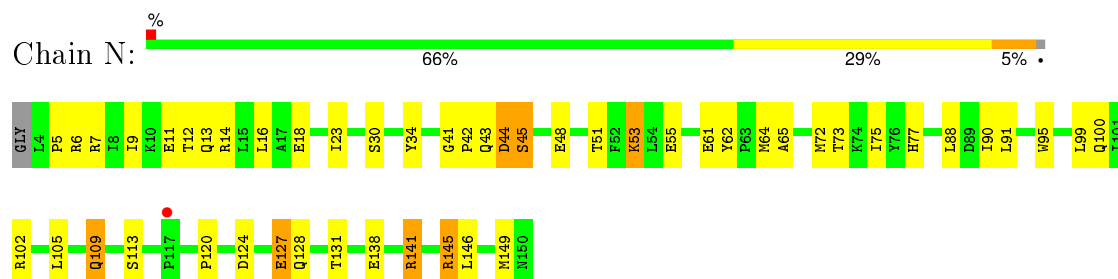
Chain J:  74% 22% ..



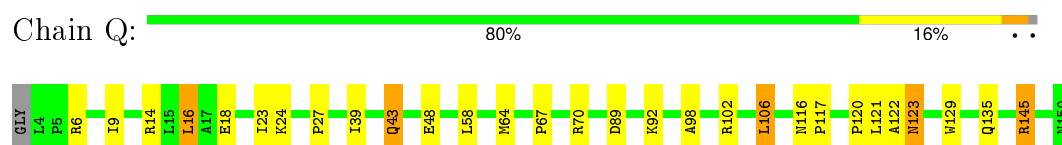
- Molecule 3: Ubiquitin-conjugating enzyme E2 N



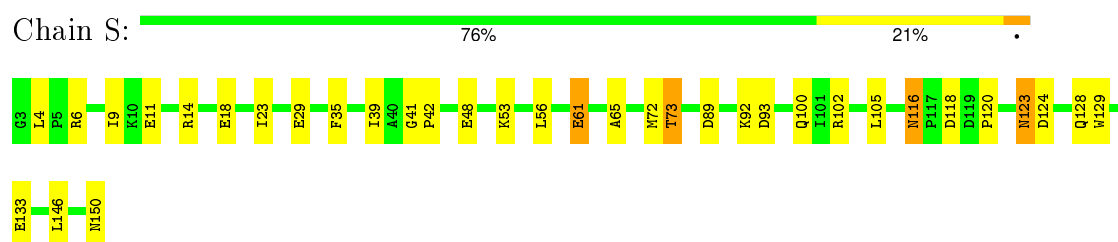
- Molecule 3: Ubiquitin-conjugating enzyme E2 N



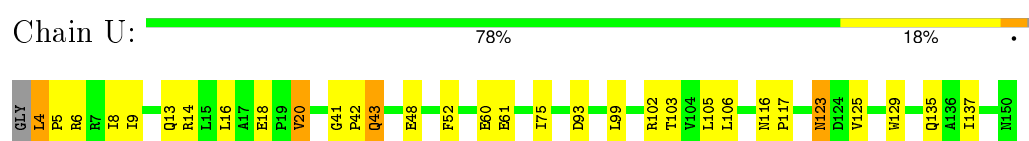
- Molecule 3: Ubiquitin-conjugating enzyme E2 N



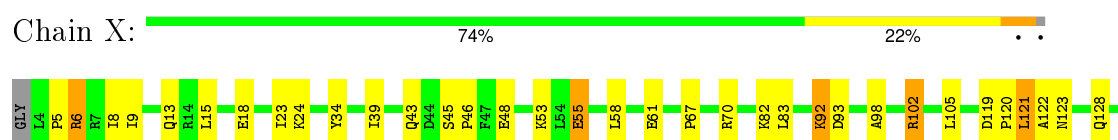
- Molecule 3: Ubiquitin-conjugating enzyme E2 N



- Molecule 3: Ubiquitin-conjugating enzyme E2 N



- Molecule 3: Ubiquitin-conjugating enzyme E2 N





- Molecule 3: Ubiquitin-conjugating enzyme E2 N

Chain Z: 81% 18% .



- Molecule 3: Ubiquitin-conjugating enzyme E2 N

Chain b: 91% 8% .



- Molecule 3: Ubiquitin-conjugating enzyme E2 N

Chain e: 88% 9% ..



- Molecule 3: Ubiquitin-conjugating enzyme E2 N

Chain g: 91% 9%



- Molecule 3: Ubiquitin-conjugating enzyme E2 N

Chain i: 91% 9%



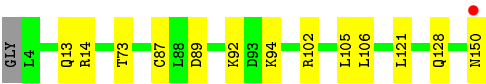
- Molecule 3: Ubiquitin-conjugating enzyme E2 N

Chain l: 89% 9% ..

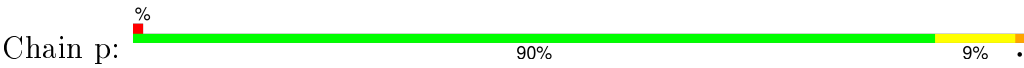


- Molecule 3: Ubiquitin-conjugating enzyme E2 N

Chain n: 91% 9% .



● Molecule 3: Ubiquitin-conjugating enzyme E2 N



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	102.06Å 137.28Å 257.11Å 90.00° 90.03° 90.00°	Depositor
Resolution (Å)	50.00 – 3.15 46.92 – 3.15	Depositor EDS
% Data completeness (in resolution range)	96.8 (50.00-3.15) 96.8 (46.92-3.15)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.22 (at 3.12Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.223 , 0.281 0.223 , 0.280	Depositor DCC
$R_{free}$ test set	6185 reflections (5.48%)	DCC
Wilson B-factor (Å <sup>2</sup> )	63.3	Xtriage
Anisotropy	0.055	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 13.8	EDS
Estimated twinning fraction	0.427 for h,-k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	11 of 118801 reflections (0.009%)	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	51450	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 51.65 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 5.4409e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.36	0/1769	0.48	0/2381
1	H	0.35	0/1806	0.49	0/2434
1	O	0.36	0/1826	0.47	0/2457
1	V	0.36	0/1816	0.48	0/2444
1	c	0.36	0/1824	0.49	0/2458
1	j	0.35	0/1768	0.47	0/2381
2	B	0.34	0/1119	0.50	0/1512
2	D	0.32	0/1115	0.51	0/1507
2	F	0.37	0/1119	0.54	0/1512
2	I	0.35	0/1119	0.54	0/1512
2	K	0.34	0/1119	0.53	0/1512
2	M	0.34	0/1119	0.52	0/1512
2	P	0.35	0/1119	0.53	0/1512
2	R	0.34	0/1115	0.52	0/1507
2	T	0.34	0/1119	0.51	0/1512
2	W	0.36	0/1115	0.52	0/1507
2	Y	0.33	0/1115	0.52	0/1507
2	a	0.34	0/1119	0.53	0/1512
2	d	0.34	0/1119	0.51	0/1512
2	f	0.32	0/1115	0.53	0/1507
2	h	0.38	0/1119	0.52	0/1512
2	k	0.35	0/1119	0.54	0/1512
2	m	0.34	0/1115	0.52	0/1507
2	o	0.34	0/1119	0.50	0/1512
3	C	0.35	0/1205	0.57	1/1640 (0.1%)
3	E	0.33	0/1205	0.55	1/1640 (0.1%)
3	G	0.36	0/1205	0.59	1/1640 (0.1%)
3	J	0.34	0/1205	0.54	0/1640
3	L	0.34	0/1205	0.53	0/1640
3	N	0.36	0/1205	0.55	0/1640
3	Q	0.34	0/1205	0.59	1/1640 (0.1%)
3	S	0.34	0/1209	0.50	0/1645
3	U	0.35	0/1205	0.55	1/1640 (0.1%)
3	X	0.34	0/1205	0.55	0/1640

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
3	Z	0.35	0/1209	0.54	0/1645
3	b	0.35	0/1205	0.52	0/1640
3	e	0.34	0/1205	0.58	2/1640 (0.1%)
3	g	0.34	0/1209	0.50	0/1645
3	i	0.36	0/1209	0.54	0/1645
3	l	0.33	0/1205	0.55	1/1640 (0.1%)
3	n	0.32	0/1205	0.51	0/1640
3	p	0.35	0/1209	0.55	1/1645 (0.1%)
All	All	0.35	0/52637	0.52	9/71286 (0.0%)

There are no bond length outliers.

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	121	LEU	CA-CB-CG	7.25	131.98	115.30
3	C	106	LEU	CA-CB-CG	6.32	129.83	115.30
3	l	106	LEU	CA-CB-CG	6.17	129.50	115.30
3	e	106	LEU	CA-CB-CG	6.05	129.21	115.30
3	e	146	LEU	CA-CB-CG	5.66	128.33	115.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1731	0	1689	18	0
1	H	1767	0	1715	15	0
1	O	1786	0	1742	17	0
1	V	1777	0	1733	18	0
1	c	1785	0	1737	0	0
1	j	1730	0	1694	0	0
2	B	1096	0	1099	6	0
2	D	1092	0	1096	20	0
2	F	1096	0	1099	24	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	I	1096	0	1099	26	0
2	K	1096	0	1099	29	0
2	M	1096	0	1099	21	0
2	P	1096	0	1099	6	0
2	R	1092	0	1096	9	0
2	T	1096	0	1099	7	0
2	W	1092	0	1096	13	0
2	Y	1092	0	1096	9	0
2	a	1096	0	1099	0	0
2	d	1096	0	1099	0	0
2	f	1092	0	1096	0	0
2	h	1096	0	1099	0	0
2	k	1096	0	1099	0	0
2	m	1092	0	1096	0	0
2	o	1096	0	1099	0	0
3	C	1175	0	1188	29	0
3	E	1175	0	1188	33	0
3	G	1175	0	1188	44	0
3	J	1175	0	1188	24	0
3	L	1175	0	1188	28	0
3	N	1175	0	1188	31	0
3	Q	1175	0	1188	14	0
3	S	1179	0	1191	15	0
3	U	1175	0	1188	14	0
3	X	1175	0	1188	19	0
3	Z	1179	0	1191	11	0
3	b	1175	0	1188	0	0
3	e	1175	0	1188	0	0
3	g	1179	0	1191	0	0
3	i	1179	0	1191	0	0
3	l	1175	0	1188	0	0
3	n	1175	0	1188	0	0
3	p	1179	0	1191	0	0
All	All	51450	0	51473	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 6.

The worst 5 of 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)
3:G:119:ASP:HB3	3:G:120:PRO:HD2	1.25	1.10
3:E:14:ARG:HG2	3:E:14:ARG:HH11	1.11	1.09
2:D:61:ARG:HD3	2:D:139:GLU:HG3	3.72	0.96
3:N:23:ILE:HD11	3:N:109:GLN:HG3	1.50	0.93
3:S:53:LYS:HG3	3:S:72:MET:HB2	1.52	0.92

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	204/228 (90%)	195 (96%)	8 (4%)	1 (0%)	34	76
1	H	208/228 (91%)	199 (96%)	7 (3%)	2 (1%)	19	63
1	O	210/228 (92%)	202 (96%)	7 (3%)	1 (0%)	34	76
1	V	209/228 (92%)	201 (96%)	7 (3%)	1 (0%)	34	76
1	c	211/228 (92%)	200 (95%)	9 (4%)	2 (1%)	21	65
1	j	204/228 (90%)	190 (93%)	11 (5%)	3 (2%)	13	53
2	B	136/138 (99%)	134 (98%)	2 (2%)	0	100	100
2	D	135/138 (98%)	129 (96%)	5 (4%)	1 (1%)	26	71
2	F	136/138 (99%)	130 (96%)	4 (3%)	2 (2%)	13	53
2	I	136/138 (99%)	122 (90%)	11 (8%)	3 (2%)	8	43
2	K	136/138 (99%)	132 (97%)	4 (3%)	0	100	100
2	M	136/138 (99%)	133 (98%)	2 (2%)	1 (1%)	26	71
2	P	136/138 (99%)	128 (94%)	6 (4%)	2 (2%)	13	53
2	R	135/138 (98%)	129 (96%)	6 (4%)	0	100	100
2	T	136/138 (99%)	128 (94%)	5 (4%)	3 (2%)	8	43
2	W	135/138 (98%)	129 (96%)	5 (4%)	1 (1%)	26	71

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	Y	135/138 (98%)	130 (96%)	4 (3%)	1 (1%)	26	71
2	a	136/138 (99%)	128 (94%)	5 (4%)	3 (2%)	8	43
2	d	136/138 (99%)	133 (98%)	2 (2%)	1 (1%)	26	71
2	f	135/138 (98%)	129 (96%)	5 (4%)	1 (1%)	26	71
2	h	136/138 (99%)	132 (97%)	3 (2%)	1 (1%)	26	71
2	k	136/138 (99%)	127 (93%)	9 (7%)	0	100	100
2	m	135/138 (98%)	130 (96%)	5 (4%)	0	100	100
2	o	136/138 (99%)	131 (96%)	3 (2%)	2 (2%)	13	53
3	C	145/148 (98%)	135 (93%)	7 (5%)	3 (2%)	9	44
3	E	145/148 (98%)	137 (94%)	8 (6%)	0	100	100
3	G	145/148 (98%)	134 (92%)	9 (6%)	2 (1%)	14	55
3	J	145/148 (98%)	136 (94%)	9 (6%)	0	100	100
3	L	145/148 (98%)	139 (96%)	6 (4%)	0	100	100
3	N	145/148 (98%)	136 (94%)	7 (5%)	2 (1%)	14	55
3	Q	145/148 (98%)	135 (93%)	8 (6%)	2 (1%)	14	55
3	S	146/148 (99%)	142 (97%)	3 (2%)	1 (1%)	26	71
3	U	145/148 (98%)	136 (94%)	9 (6%)	0	100	100
3	X	145/148 (98%)	135 (93%)	8 (6%)	2 (1%)	14	55
3	Z	146/148 (99%)	142 (97%)	4 (3%)	0	100	100
3	b	145/148 (98%)	135 (93%)	10 (7%)	0	100	100
3	e	145/148 (98%)	136 (94%)	7 (5%)	2 (1%)	14	55
3	g	146/148 (99%)	140 (96%)	6 (4%)	0	100	100
3	i	146/148 (99%)	135 (92%)	11 (8%)	0	100	100
3	l	145/148 (98%)	134 (92%)	11 (8%)	0	100	100
3	n	145/148 (98%)	139 (96%)	6 (4%)	0	100	100
3	p	146/148 (99%)	136 (93%)	10 (7%)	0	100	100
All	All	6303/6516 (97%)	5983 (95%)	274 (4%)	46 (1%)	26	71

5 of 46 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	F	93	ASN
1	H	152	GLN

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Mol	Chain	Res	Type
2	I	107	ALA
2	T	93	ASN
1	V	152	GLN

### 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	193/207 (93%)	178 (92%)	15 (8%)	16	51
1	H	197/207 (95%)	177 (90%)	20 (10%)	9	35
1	O	198/207 (96%)	182 (92%)	16 (8%)	15	49
1	V	198/207 (96%)	190 (96%)	8 (4%)	38	76
1	c	199/207 (96%)	183 (92%)	16 (8%)	15	50
1	j	193/207 (93%)	176 (91%)	17 (9%)	12	43
2	B	123/123 (100%)	116 (94%)	7 (6%)	25	65
2	D	123/123 (100%)	115 (94%)	8 (6%)	21	60
2	F	123/123 (100%)	113 (92%)	10 (8%)	15	49
2	I	123/123 (100%)	104 (85%)	19 (15%)	3	15
2	K	123/123 (100%)	115 (94%)	8 (6%)	21	60
2	M	123/123 (100%)	112 (91%)	11 (9%)	12	42
2	P	123/123 (100%)	112 (91%)	11 (9%)	12	42
2	R	123/123 (100%)	121 (98%)	2 (2%)	70	90
2	T	123/123 (100%)	110 (89%)	13 (11%)	8	33
2	W	123/123 (100%)	110 (89%)	13 (11%)	8	33
2	Y	123/123 (100%)	117 (95%)	6 (5%)	31	71
2	a	123/123 (100%)	116 (94%)	7 (6%)	25	65
2	d	123/123 (100%)	115 (94%)	8 (6%)	21	60
2	f	123/123 (100%)	111 (90%)	12 (10%)	10	37
2	h	123/123 (100%)	115 (94%)	8 (6%)	21	60

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	k	123/123 (100%)	110 (89%)	13 (11%)	8	33
2	m	123/123 (100%)	118 (96%)	5 (4%)	37	75
2	o	123/123 (100%)	115 (94%)	8 (6%)	21	60
3	C	126/126 (100%)	105 (83%)	21 (17%)	3	12
3	E	126/126 (100%)	113 (90%)	13 (10%)	9	34
3	G	126/126 (100%)	112 (89%)	14 (11%)	8	31
3	J	126/126 (100%)	113 (90%)	13 (10%)	9	34
3	L	126/126 (100%)	113 (90%)	13 (10%)	9	34
3	N	126/126 (100%)	112 (89%)	14 (11%)	8	31
3	Q	126/126 (100%)	113 (90%)	13 (10%)	9	34
3	S	126/126 (100%)	111 (88%)	15 (12%)	6	27
3	U	126/126 (100%)	114 (90%)	12 (10%)	11	38
3	X	126/126 (100%)	112 (89%)	14 (11%)	8	31
3	Z	126/126 (100%)	113 (90%)	13 (10%)	9	34
3	b	126/126 (100%)	114 (90%)	12 (10%)	11	38
3	e	126/126 (100%)	110 (87%)	16 (13%)	5	24
3	g	126/126 (100%)	113 (90%)	13 (10%)	9	34
3	i	126/126 (100%)	112 (89%)	14 (11%)	8	31
3	l	126/126 (100%)	111 (88%)	15 (12%)	6	27
3	n	126/126 (100%)	113 (90%)	13 (10%)	9	34
3	p	126/126 (100%)	111 (88%)	15 (12%)	6	27
All	All	5660/5724 (99%)	5146 (91%)	514 (9%)	12	41

5 of 514 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	S	73	THR
2	W	133	LYS
2	m	31	VAL
3	S	124	ASP
3	U	93	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 98 such sidechains are listed below:

Mol	Chain	Res	Type
2	R	120	GLN
1	V	70	GLN
3	I	109	GLN
3	S	13	GLN
2	T	120	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

### 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

### 5.5 Carbohydrates [i](#)

There are no 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](#)

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	210/228 (92%)	0.03	1 (0%) 91 87	58, 87, 128, 158	0
1	H	214/228 (93%)	0.62	20 (9%) 11 5	95, 129, 181, 205	0
1	O	216/228 (94%)	-0.02	1 (0%) 91 87	59, 78, 110, 142	0
1	V	215/228 (94%)	-0.05	2 (0%) 85 77	57, 78, 113, 153	0
1	c	217/228 (95%)	0.07	8 (3%) 45 28	58, 87, 133, 174	0
1	j	210/228 (92%)	0.62	21 (10%) 9 4	97, 131, 177, 194	0
2	B	138/138 (100%)	-0.39	1 (0%) 89 82	47, 62, 80, 106	0
2	D	137/138 (99%)	-0.27	0 100 100	59, 84, 113, 138	0
2	F	138/138 (100%)	-0.34	0 100 100	42, 57, 83, 102	0
2	I	138/138 (100%)	-0.08	0 100 100	61, 88, 118, 152	0
2	K	138/138 (100%)	-0.34	1 (0%) 89 82	53, 67, 82, 99	0
2	M	138/138 (100%)	-0.34	0 100 100	51, 66, 86, 113	0
2	P	138/138 (100%)	-0.03	1 (0%) 89 82	71, 98, 131, 153	0
2	R	137/138 (99%)	-0.43	0 100 100	53, 67, 84, 94	0
2	T	138/138 (100%)	-0.23	0 100 100	56, 73, 103, 132	0
2	W	137/138 (99%)	-0.11	0 100 100	69, 94, 122, 138	0
2	Y	137/138 (99%)	-0.34	0 100 100	54, 70, 87, 97	0
2	a	138/138 (100%)	-0.29	1 (0%) 89 82	53, 71, 103, 127	0
2	d	138/138 (100%)	-0.38	1 (0%) 89 82	48, 62, 81, 105	0
2	f	137/138 (99%)	-0.19	0 100 100	61, 83, 109, 131	0
2	h	138/138 (100%)	-0.36	0 100 100	42, 57, 81, 100	0
2	k	138/138 (100%)	-0.12	0 100 100	64, 89, 117, 155	0
2	m	137/138 (99%)	-0.34	0 100 100	54, 69, 84, 98	0
2	o	138/138 (100%)	-0.38	0 100 100	50, 65, 87, 107	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
3	C	147/148 (99%)	-0.30	1 (0%) 89 82	40, 63, 95, 119	0
3	E	147/148 (99%)	-0.21	0 100 100	51, 81, 135, 155	0
3	G	147/148 (99%)	-0.32	0 100 100	39, 56, 92, 104	0
3	J	147/148 (99%)	-0.14	0 100 100	57, 78, 116, 136	0
3	L	147/148 (99%)	-0.20	2 (1%) 78 64	54, 83, 138, 167	0
3	N	147/148 (99%)	-0.28	1 (0%) 89 82	54, 68, 97, 106	0
3	Q	147/148 (99%)	-0.33	0 100 100	49, 65, 95, 109	0
3	S	148/148 (100%)	-0.30	0 100 100	49, 75, 103, 115	0
3	U	147/148 (99%)	-0.28	0 100 100	50, 66, 98, 114	0
3	X	147/148 (99%)	-0.31	0 100 100	50, 67, 98, 110	0
3	Z	148/148 (100%)	-0.24	0 100 100	49, 75, 105, 116	0
3	b	147/148 (99%)	-0.30	0 100 100	49, 66, 96, 113	0
3	e	147/148 (99%)	-0.27	1 (0%) 89 82	40, 63, 96, 108	0
3	g	148/148 (100%)	-0.17	1 (0%) 89 82	48, 81, 137, 158	0
3	i	148/148 (100%)	-0.28	1 (0%) 89 82	39, 57, 93, 111	0
3	l	147/148 (99%)	-0.20	1 (0%) 89 82	57, 82, 121, 145	0
3	n	147/148 (99%)	-0.12	1 (0%) 89 82	58, 86, 140, 166	0
3	p	148/148 (100%)	-0.24	1 (0%) 89 82	55, 70, 101, 115	0
All	All	6411/6516 (98%)	-0.17	68 (1%) 82 71	39, 74, 129, 205	0

The worst 5 of 68 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	68	TYR	5.7
1	j	57	LEU	5.6
1	H	57	LEU	5.6
1	c	242	GLY	4.7
2	K	6	GLY	4.7

## 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 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.