



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 10, 2018 – 12:54 pm GMT

PDB ID : 3D29  
Title : Proteasome Inhibition by Fellutamide B  
Authors : Groll, M.; Hines, J.; Fahnestock, M.; Crews, M.C.  
Deposited on : 2008-05-07  
Resolution : 2.60 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7.3 (157068), CSD as539be (2018)  
Xtriage (Phenix) : 1.13  
EDS : trunk30967  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk30967

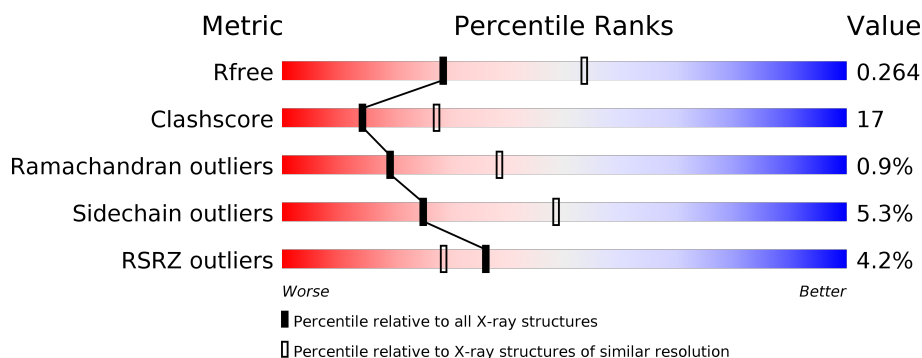
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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))
$R_{free}$	111664	2767 (2.60-2.60)
Clashscore	122126	3110 (2.60-2.60)
Ramachandran outliers	120053	3062 (2.60-2.60)
Sidechain outliers	120020	3062 (2.60-2.60)
RSRZ outliers	108989	2706 (2.60-2.60)

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	250	<div> <div>4%</div> <div>74%</div> <div>24%</div> <div>•</div> </div>
1	O	250	<div> <div>6%</div> <div>75%</div> <div>24%</div> <div>•</div> </div>
2	B	244	<div> <div>6%</div> <div>59%</div> <div>37%</div> <div>•</div> </div>
2	P	244	<div> <div>6%</div> <div>57%</div> <div>40%</div> <div>•</div> </div>
3	C	241	<div> <div>11%</div> <div>61%</div> <div>37%</div> <div>•</div> </div>
3	Q	241	<div> <div>15%</div> <div>61%</div> <div>37%</div> <div>•</div> </div>

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Mol	Chain	Length	Quality of chain
4	D	242	
4	R	242	
5	E	233	
5	S	233	
6	F	244	
6	T	244	
7	G	243	
7	U	243	
8	H	222	
8	V	222	
9	I	204	
9	W	204	
10	J	198	
10	X	198	
11	K	212	
11	Y	212	
12	L	222	
12	Z	222	
13	1	233	
13	M	233	
14	2	196	
14	N	196	

## 2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 51114 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 Proteasome component Y7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	250	Total	C	N	O	S	0	0	0
			1915	1219	315	377	4			
1	O	250	Total	C	N	O	S	0	0	0
			1915	1219	315	377	4			

- Molecule 2 is a protein called Proteasome component Y13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	244	Total	C	N	O	S	0	0	0
			1905	1201	321	380	3			
2	P	244	Total	C	N	O	S	0	0	0
			1905	1201	321	380	3			

- Molecule 3 is a protein called Proteasome component PRE6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	241	Total	C	N	O	S	0	0	0
			1891	1181	331	375	4			
3	Q	241	Total	C	N	O	S	0	0	0
			1891	1181	331	375	4			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	237	GLU	-	EXPRESSION TAG	UNP P40303
C	238	GLN	-	EXPRESSION TAG	UNP P40303
C	239	GLU	-	EXPRESSION TAG	UNP P40303
C	240	LYS	-	EXPRESSION TAG	UNP P40303
C	241	GLN	-	EXPRESSION TAG	UNP P40303
C	242	GLU	-	EXPRESSION TAG	UNP P40303
C	243	GLN	-	EXPRESSION TAG	UNP P40303
Q	237	GLU	-	EXPRESSION TAG	UNP P40303

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Chain	Residue	Modelled	Actual	Comment	Reference
Q	238	GLN	-	EXPRESSION TAG	UNP P40303
Q	239	GLU	-	EXPRESSION TAG	UNP P40303
Q	240	LYS	-	EXPRESSION TAG	UNP P40303
Q	241	GLN	-	EXPRESSION TAG	UNP P40303
Q	242	GLU	-	EXPRESSION TAG	UNP P40303
Q	243	GLN	-	EXPRESSION TAG	UNP P40303

- Molecule 4 is a protein called Proteasome component PUP2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	242	Total	C	N	O	S	0	0	0
			1862	1162	314	379	7			
4	R	242	Total	C	N	O	S	0	0	0
			1862	1162	314	379	7			

- Molecule 5 is a protein called Proteasome component PRE5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	233	Total	C	N	O	S	0	0	0
			1795	1129	312	350	4			
5	S	233	Total	C	N	O	S	0	0	0
			1795	1129	312	350	4			

- Molecule 6 is a protein called Proteasome component C1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	244	Total	C	N	O	S	0	0	0
			1897	1205	330	358	4			
6	T	244	Total	C	N	O	S	0	0	0
			1897	1205	330	358	4			

- Molecule 7 is a protein called Proteasome component C7-alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	243	Total	C	N	O	S	0	0	0
			1921	1221	322	370	8			
7	U	243	Total	C	N	O	S	0	0	0
			1921	1221	322	370	8			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	6	ALA	-	EXPRESSION TAG	UNP P21243
G	7	GLY	-	EXPRESSION TAG	UNP P21243
U	6	ALA	-	EXPRESSION TAG	UNP P21243
U	7	GLY	-	EXPRESSION TAG	UNP P21243

- Molecule 8 is a protein called Proteasome component PUP1 precursor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	222	Total	C	N	O	S	0	0	0
			1685	1061	293	324	7			
8	V	222	Total	C	N	O	S	0	0	0
			1685	1061	293	324	7			

- Molecule 9 is a protein called Proteasome component PUP3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	204	Total	C	N	O	S	0	0	0
			1581	1010	258	305	8			
9	W	204	Total	C	N	O	S	0	0	0
			1581	1010	258	305	8			

- Molecule 10 is a protein called Proteasome component C11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	198	Total	C	N	O	S	0	0	0
			1585	1005	269	305	6			
10	X	198	Total	C	N	O	S	0	0	0
			1585	1005	269	305	6			

- Molecule 11 is a protein called Proteasome component PRE2 precursor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	212	Total	C	N	O	S	0	0	0
			1644	1045	280	312	7			
11	Y	212	Total	C	N	O	S	0	0	0
			1644	1045	280	312	7			

- Molecule 12 is a protein called Proteasome component C5 precursor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	222	Total	C	N	O	S	0	0	0
			1757	1115	303	335	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	Z	222	Total	C	N	O	S	0	0	0
			1757	1115	303	335	4			

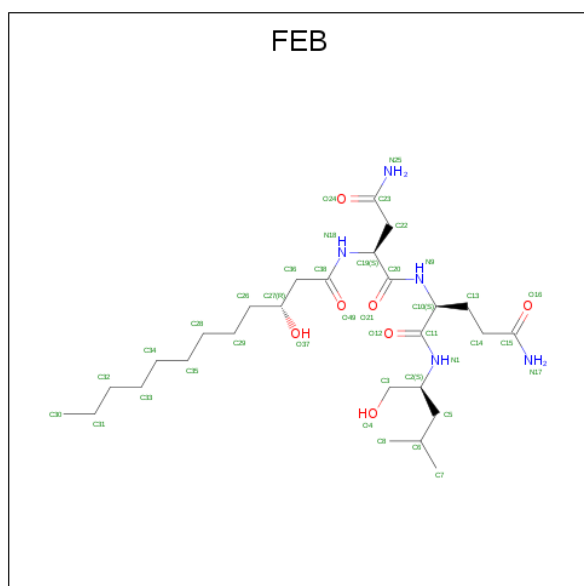
- Molecule 13 is a protein called Proteasome component PRE4 precursor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	233	Total	C	N	O	S	0	0	0
			1824	1154	312	351	7			
13	1	233	Total	C	N	O	S	0	0	0
			1824	1154	312	351	7			

- Molecule 14 is a protein called Proteasome component PRE3 precursor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	N	196	Total	C	N	O	S	0	0	0
			1512	955	250	300	7			
14	2	196	Total	C	N	O	S	0	0	0
			1512	955	250	300	7			

- Molecule 15 is N 2 -[(3R)-3-hydroxydodecanoyl]-L-asparaginyl-N 1 -[(1S)-1-(hydroxymethyl)-3-methylbutyl]-L-glutamamide (three-letter code: FEB) (formula: C<sub>27</sub>H<sub>51</sub>N<sub>5</sub>O<sub>7</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
15	H	1	Total	C	N	O	0	0
			39	27	5	7		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
15	K	1	Total	C	N	O	0	0
			39	27	5	7		
15	N	1	Total	C	N	O	0	0
			39	27	5	7		
15	V	1	Total	C	N	O	0	0
			39	27	5	7		
15	Y	1	Total	C	N	O	0	0
			39	27	5	7		
15	2	1	Total	C	N	O	0	0
			39	27	5	7		

- Molecule 16 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	A	55	Total	O	0	0
			55	55		
16	B	36	Total	O	0	0
			36	36		
16	C	46	Total	O	0	0
			46	46		
16	D	42	Total	O	0	0
			42	42		
16	E	23	Total	O	0	0
			23	23		
16	F	46	Total	O	0	0
			46	46		
16	G	62	Total	O	0	0
			62	62		
16	H	51	Total	O	0	0
			51	51		
16	I	66	Total	O	0	0
			66	66		
16	J	53	Total	O	0	0
			53	53		
16	K	42	Total	O	0	0
			42	42		
16	L	56	Total	O	0	0
			56	56		
16	M	68	Total	O	0	0
			68	68		
16	N	59	Total	O	0	0
			59	59		

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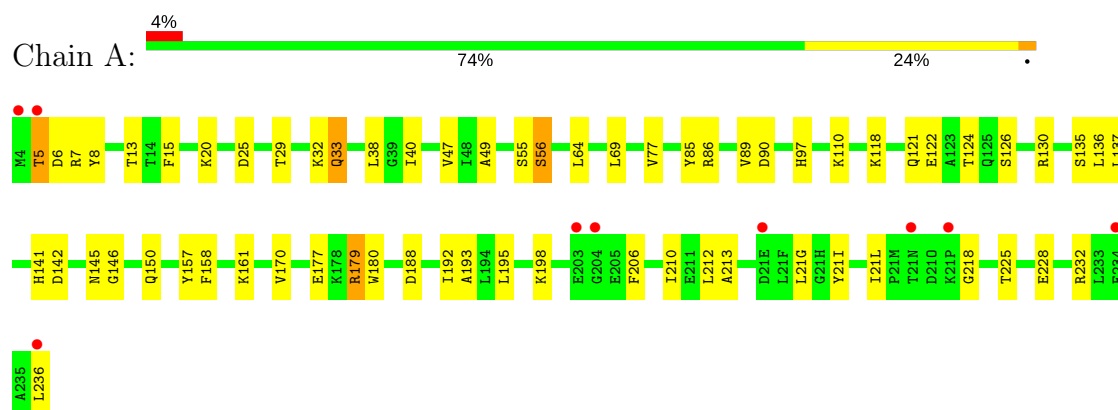
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	O	35	Total 35	O 35	0	0
16	P	29	Total 29	O 29	0	0
16	Q	26	Total 26	O 26	0	0
16	R	31	Total 31	O 31	0	0
16	S	20	Total 20	O 20	0	0
16	T	39	Total 39	O 39	0	0
16	U	61	Total 61	O 61	0	0
16	V	48	Total 48	O 48	0	0
16	W	59	Total 59	O 59	0	0
16	X	46	Total 46	O 46	0	0
16	Y	48	Total 48	O 48	0	0
16	Z	52	Total 52	O 52	0	0
16	1	74	Total 74	O 74	0	0
16	2	59	Total 59	O 59	0	0

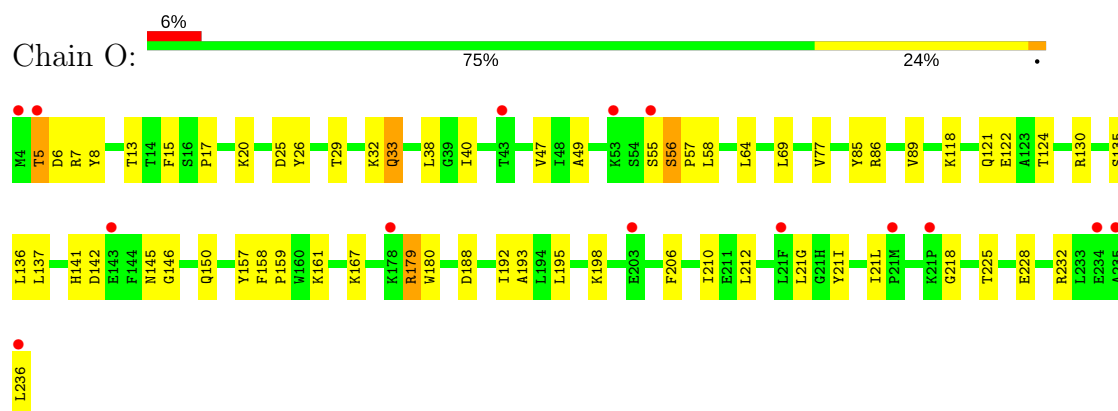
### 3 Residue-property plots

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

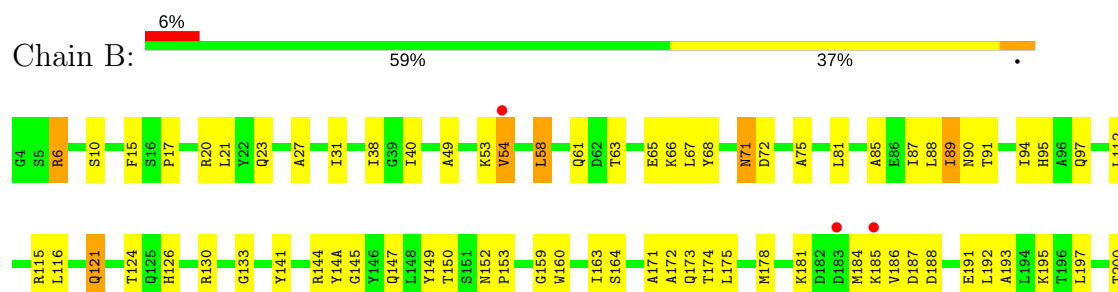
#### • Molecule 1: Proteasome component Y7

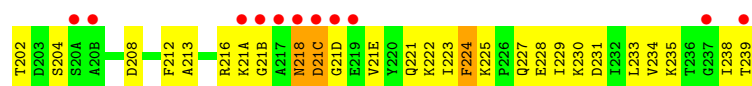


#### • Molecule 1: Proteasome component Y7

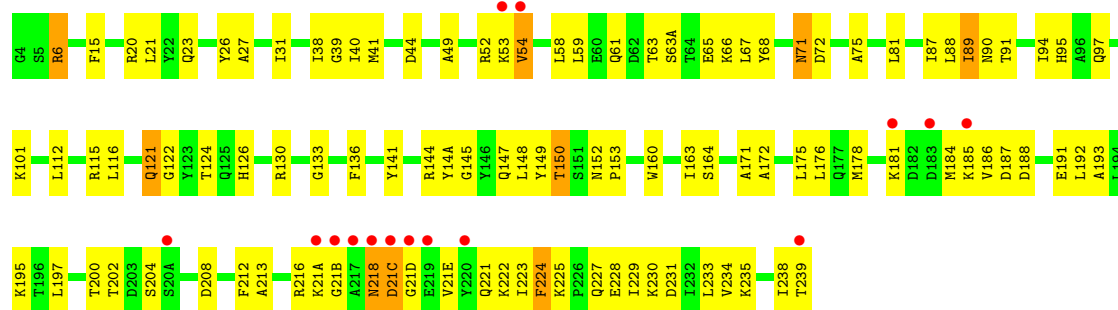


#### • Molecule 2: Proteasome component Y13

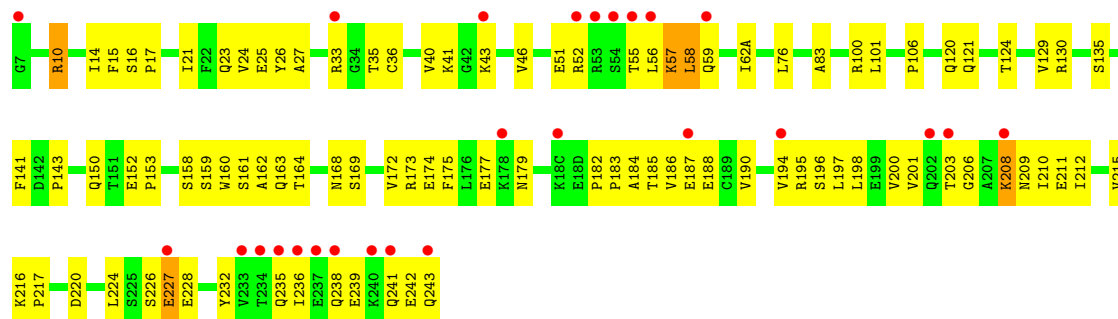




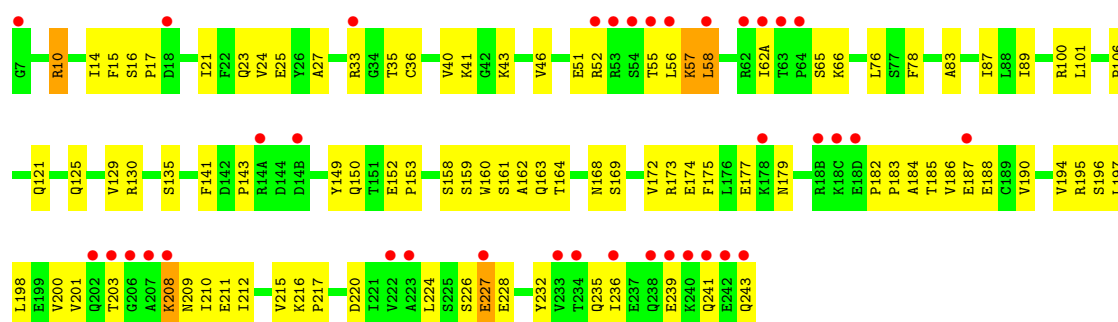
• Molecule 2: Proteasome component Y13



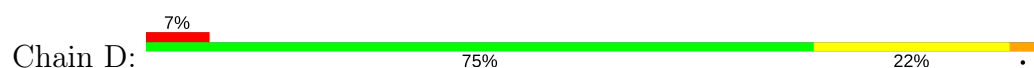
• Molecule 3: Proteasome component PRE6

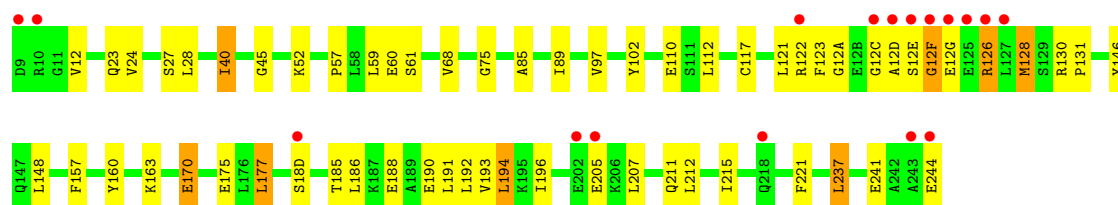


• Molecule 3: Proteasome component PRE6

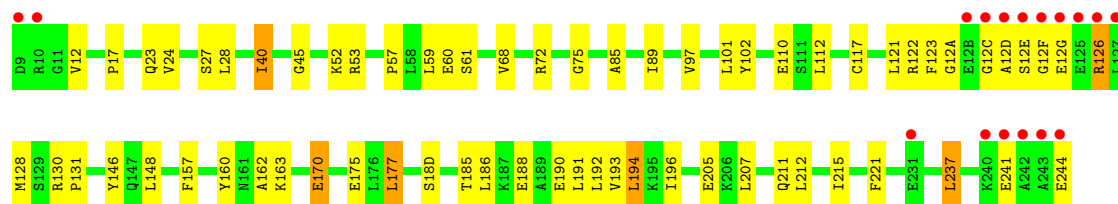
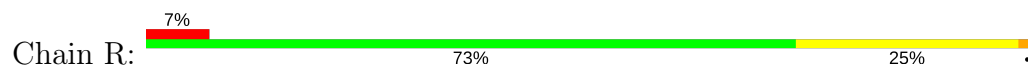


• Molecule 4: Proteasome component PUP2

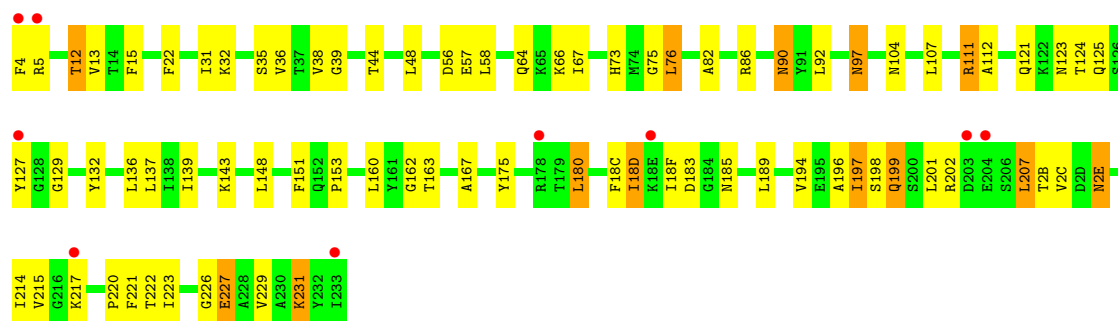




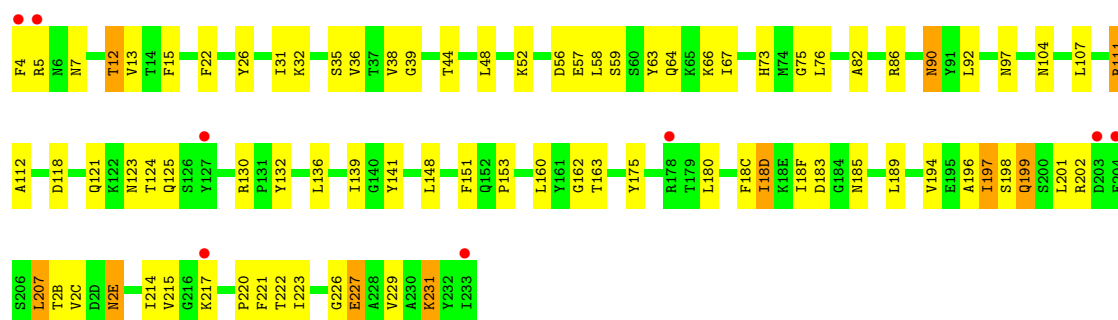
• Molecule 4: Proteasome component PUP2



• Molecule 5: Proteasome component PRE5

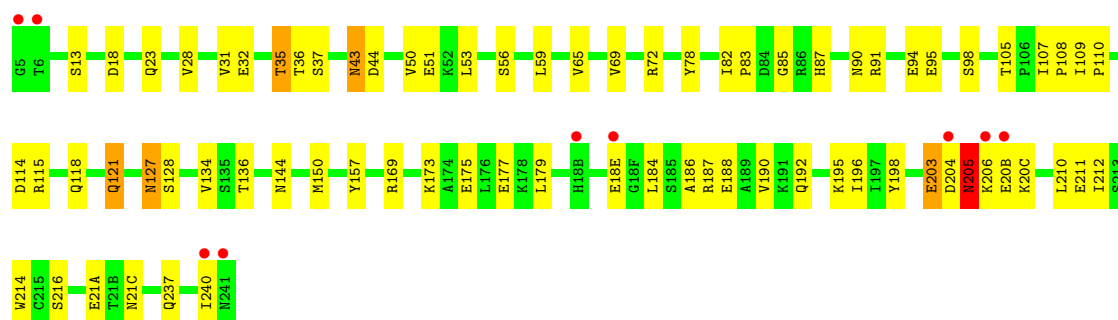


• Molecule 5: Proteasome component PRE5

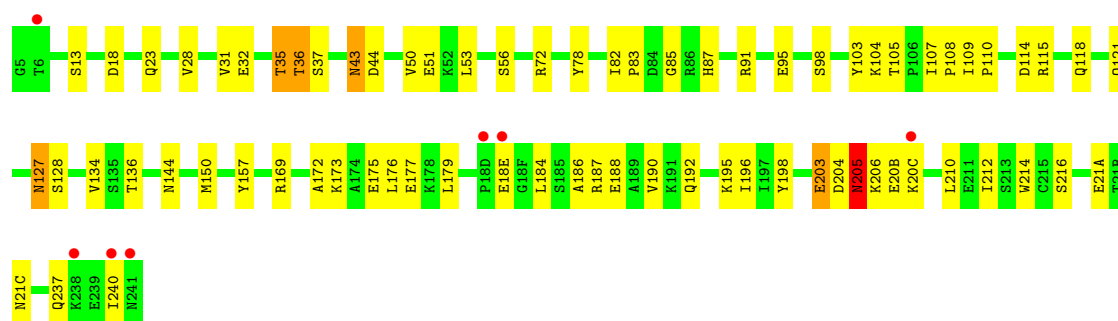


• Molecule 6: Proteasome component C1

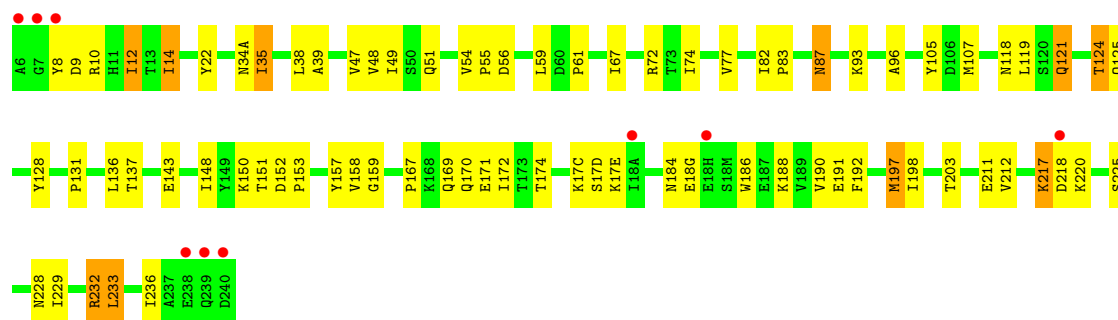




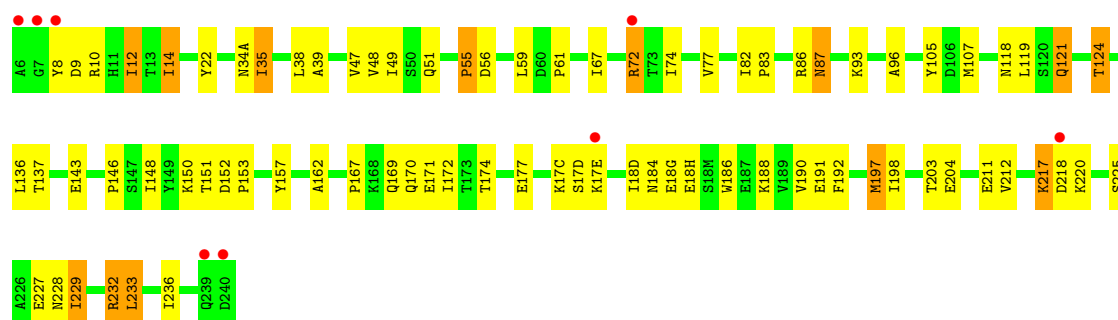
• Molecule 6: Proteasome component C1



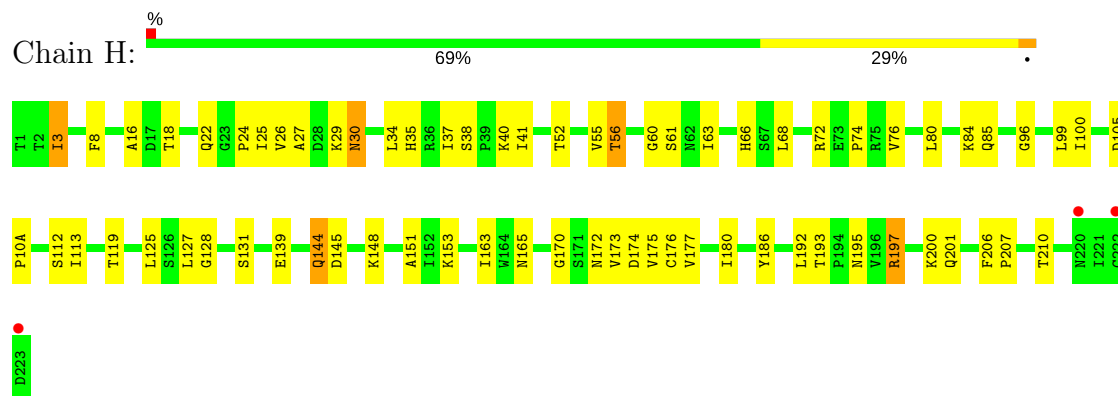
• Molecule 7: Proteasome component C7-alpha



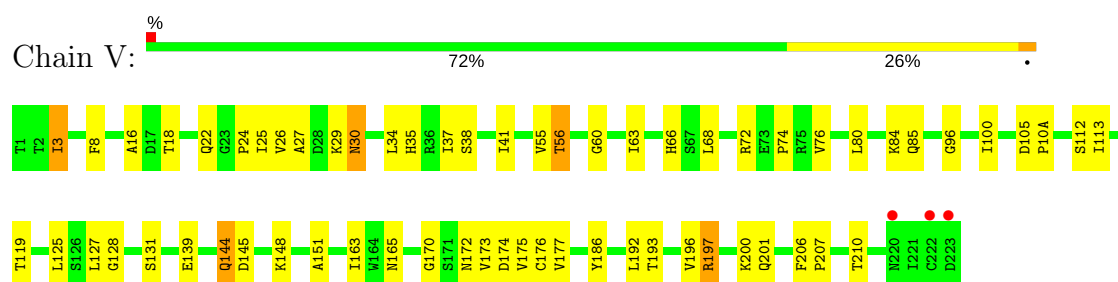
• Molecule 7: Proteasome component C7-alpha



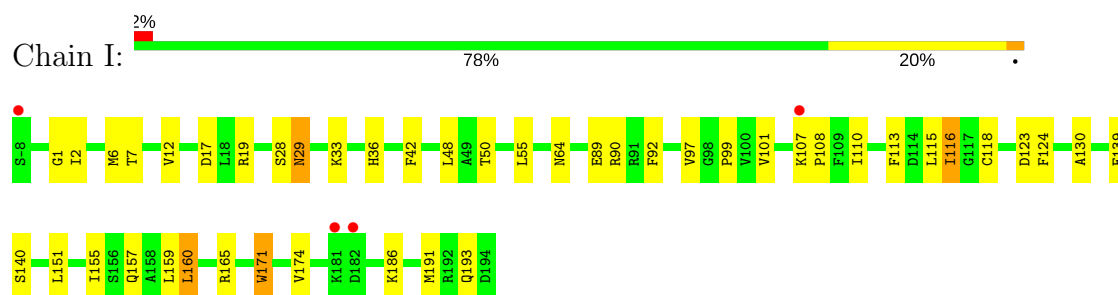
- Molecule 8: Proteasome component PUP1 precursor



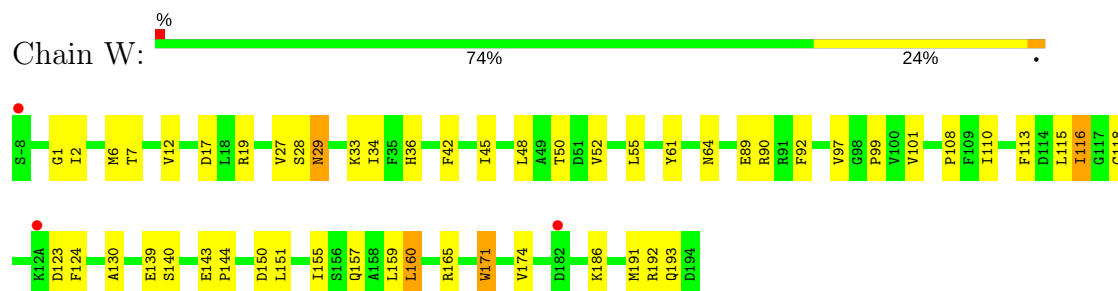
- Molecule 8: Proteasome component PUP1 precursor



- Molecule 9: Proteasome component PUP3

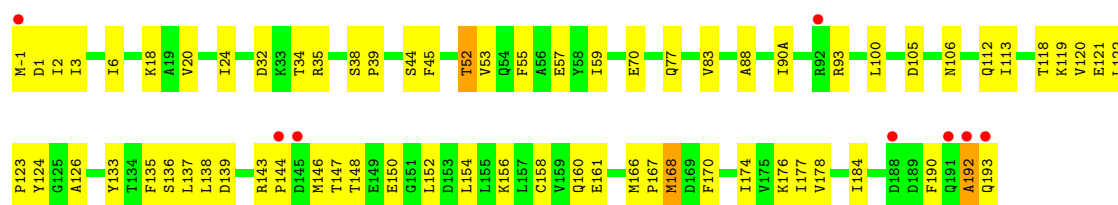


- Molecule 9: Proteasome component PUP3



- Molecule 10: Proteasome component C11

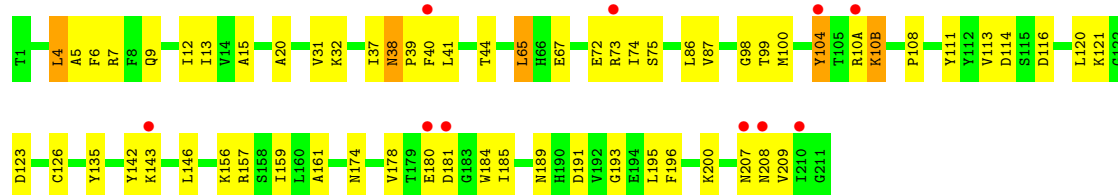




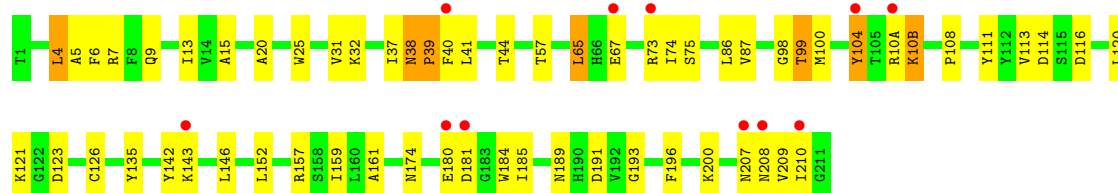
• Molecule 10: Proteasome component C11



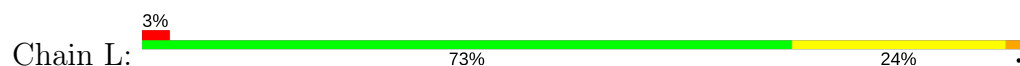
• Molecule 11: Proteasome component PRE2 precursor

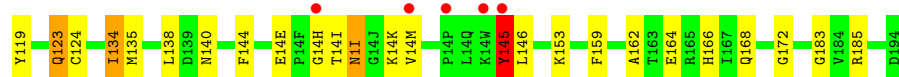


• Molecule 11: Proteasome component PRE2 precursor

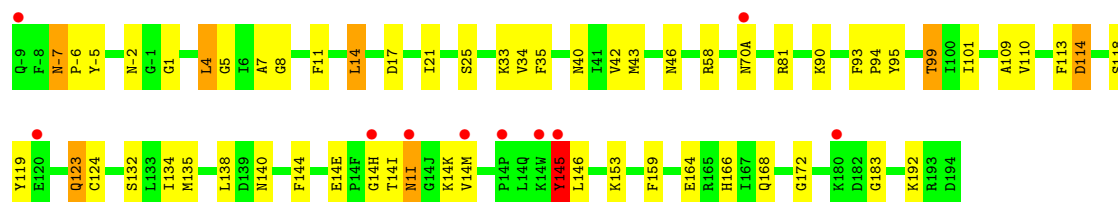


• Molecule 12: Proteasome component C5 precursor

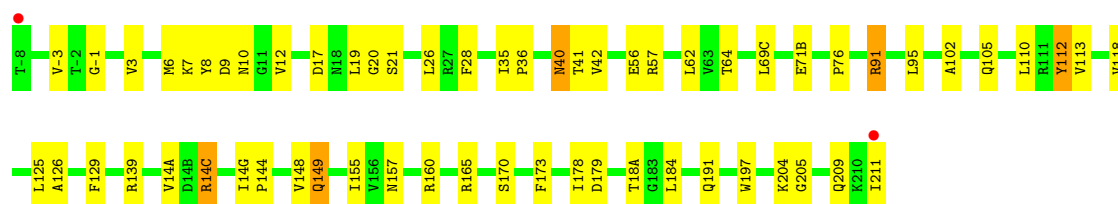
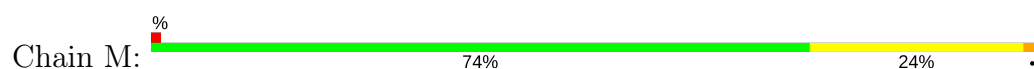




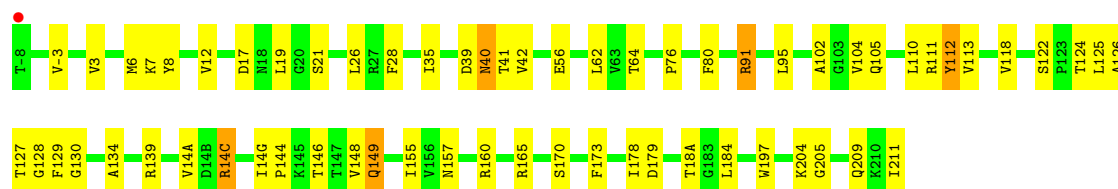
- Molecule 12: Proteasome component C5 precursor



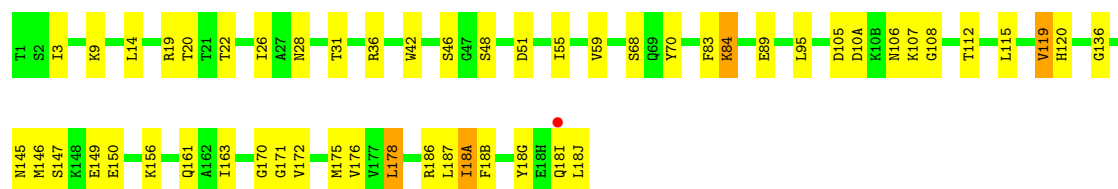
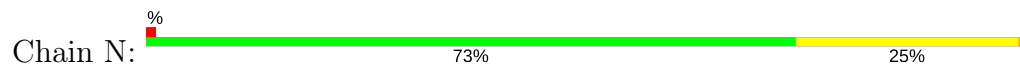
- Molecule 13: Proteasome component PRE4 precursor



- Molecule 13: Proteasome component PRE4 precursor



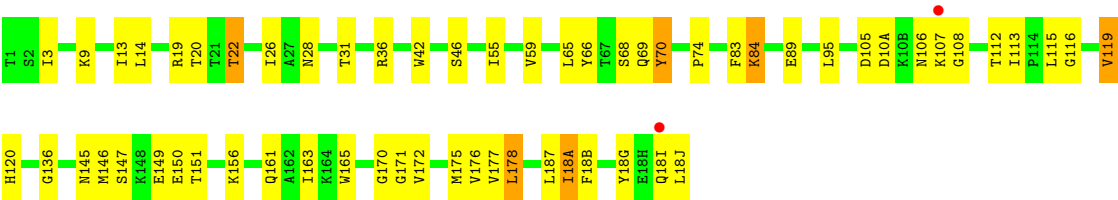
- Molecule 14: Proteasome component PRE3 precursor



- Molecule 14: Proteasome component PRE3 precursor







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	134.27Å 301.58Å 143.45Å 90.00° 112.70° 90.00°	Depositor
Resolution (Å)	15.00 – 2.60 19.99 – 2.56	Depositor EDS
% Data completeness (in resolution range)	98.2 (15.00-2.60) 98.0 (19.99-2.56)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.15 (at 2.56Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.240 , 0.266 0.239 , 0.264	Depositor DCC
$R_{free}$ test set	15699 reflections (4.79%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	47.3	Xtriage
Anisotropy	0.795	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 59.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.52$ , $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	51114	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.66% 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](#)

Bond lengths and bond angles in the following residue types are not validated in this section: FEB

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	0.38	0/1952	0.63	0/2642
1	O	0.38	0/1952	0.63	0/2642
2	B	0.35	0/1935	0.62	0/2618
2	P	0.36	0/1935	0.62	0/2618
3	C	0.35	0/1920	0.60	0/2598
3	Q	0.35	0/1920	0.61	0/2598
4	D	0.35	0/1887	0.62	0/2541
4	R	0.35	0/1887	0.62	0/2541
5	E	0.36	0/1823	0.62	0/2463
5	S	0.36	0/1823	0.62	0/2463
6	F	0.38	0/1937	0.62	0/2614
6	T	0.39	0/1937	0.62	0/2614
7	G	0.42	0/1959	0.65	0/2652
7	U	0.41	0/1959	0.64	0/2652
8	H	0.39	0/1716	0.66	0/2326
8	V	0.39	0/1716	0.66	0/2326
9	I	0.40	0/1611	0.67	0/2174
9	W	0.41	0/1611	0.68	0/2174
10	J	0.39	0/1613	0.65	0/2173
10	X	0.39	0/1613	0.65	0/2173
11	K	0.42	0/1681	0.69	1/2274 (0.0%)
11	Y	0.43	0/1681	0.69	1/2274 (0.0%)
12	L	0.42	0/1795	0.70	1/2420 (0.0%)
12	Z	0.41	0/1795	0.69	1/2420 (0.0%)
13	1	0.40	0/1855	0.67	1/2514 (0.0%)
13	M	0.40	0/1855	0.67	1/2514 (0.0%)
14	2	0.41	0/1541	0.67	1/2087 (0.0%)
14	N	0.43	0/1541	0.67	0/2087
All	All	0.39	0/50450	0.65	7/68192 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if

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

Mol	Chain	#Chirality outliers	#Planarity outliers
12	L	0	1
12	Z	0	1
All	All	0	2

There are no bond length outliers.

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	1	95	LEU	N-CA-C	-5.53	96.07	111.00
13	M	95	LEU	N-CA-C	-5.39	96.43	111.00
14	2	22	THR	N-CA-C	-5.16	97.07	111.00
11	K	98	GLY	N-CA-C	-5.16	100.21	113.10
11	Y	98	GLY	N-CA-C	-5.14	100.25	113.10

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
12	L	145	TYR	Sidechain
12	Z	145	TYR	Sidechain

## 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	1915	0	1926	59	0
1	O	1915	0	1926	58	0
2	B	1905	0	1901	97	0
2	P	1905	0	1901	91	0
3	C	1891	0	1900	107	0
3	Q	1891	0	1900	103	0
4	D	1862	0	1836	50	0
4	R	1862	0	1836	56	0
5	E	1795	0	1797	73	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	S	1795	0	1797	70	0
6	F	1897	0	1886	60	0
6	T	1897	0	1886	54	0
7	G	1921	0	1910	78	0
7	U	1921	0	1910	80	0
8	H	1685	0	1687	62	0
8	V	1685	0	1687	54	0
9	I	1581	0	1574	50	0
9	W	1581	0	1574	53	0
10	J	1585	0	1590	63	0
10	X	1585	0	1590	65	0
11	K	1644	0	1594	70	0
11	Y	1644	0	1594	71	0
12	L	1757	0	1711	52	0
12	Z	1757	0	1711	51	0
13	1	1824	0	1832	50	0
13	M	1824	0	1832	52	0
14	2	1512	0	1480	53	0
14	N	1512	0	1480	49	0
15	2	39	0	50	6	0
15	H	39	0	50	3	0
15	K	39	0	50	0	0
15	N	39	0	50	7	0
15	V	39	0	50	3	0
15	Y	39	0	50	0	0
16	1	74	0	0	4	0
16	2	59	0	0	1	0
16	A	55	0	0	4	0
16	B	36	0	0	1	0
16	C	46	0	0	1	0
16	D	42	0	0	2	0
16	E	23	0	0	1	0
16	F	46	0	0	2	0
16	G	62	0	0	3	0
16	H	51	0	0	3	0
16	I	66	0	0	2	0
16	J	53	0	0	3	0
16	K	42	0	0	6	0
16	L	56	0	0	4	0
16	M	68	0	0	6	0
16	N	59	0	0	2	0
16	O	35	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	P	29	0	0	2	0
16	Q	26	0	0	2	0
16	R	31	0	0	3	0
16	S	20	0	0	1	0
16	T	39	0	0	2	0
16	U	61	0	0	6	0
16	V	48	0	0	3	0
16	W	59	0	0	1	0
16	X	46	0	0	6	0
16	Y	48	0	0	13	0
16	Z	52	0	0	3	0
All	All	51114	0	49548	1656	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 17.

The worst 5 of 1656 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)
11:K:10(B):LYS:H	11:K:10(B):LYS:HD2	1.10	1.16
8:V:3:ILE:HD11	8:V:127:LEU:HB2	1.33	1.10
8:H:3:ILE:HD11	8:H:127:LEU:HB2	1.33	1.10
3:Q:201:VAL:HG21	3:Q:210:ILE:HD11	1.10	1.09
11:Y:10(B):LYS:HD2	11:Y:10(B):LYS:H	1.11	1.09

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	248/250 (99%)	231 (93%)	15 (6%)	2 (1%)	21 42

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	O	248/250 (99%)	232 (94%)	13 (5%)	3 (1%)	14	30
2	B	242/244 (99%)	225 (93%)	13 (5%)	4 (2%)	10	20
2	P	242/244 (99%)	225 (93%)	13 (5%)	4 (2%)	10	20
3	C	239/241 (99%)	221 (92%)	15 (6%)	3 (1%)	13	27
3	Q	239/241 (99%)	221 (92%)	15 (6%)	3 (1%)	13	27
4	D	240/242 (99%)	221 (92%)	12 (5%)	7 (3%)	5	8
4	R	240/242 (99%)	221 (92%)	13 (5%)	6 (2%)	6	11
5	E	231/233 (99%)	214 (93%)	13 (6%)	4 (2%)	10	20
5	S	231/233 (99%)	213 (92%)	16 (7%)	2 (1%)	19	38
6	F	242/244 (99%)	230 (95%)	9 (4%)	3 (1%)	14	30
6	T	242/244 (99%)	230 (95%)	9 (4%)	3 (1%)	14	30
7	G	241/243 (99%)	229 (95%)	12 (5%)	0	100	100
7	U	241/243 (99%)	229 (95%)	11 (5%)	1 (0%)	36	60
8	H	220/222 (99%)	210 (96%)	8 (4%)	2 (1%)	19	38
8	V	220/222 (99%)	210 (96%)	9 (4%)	1 (0%)	31	56
9	I	202/204 (99%)	194 (96%)	8 (4%)	0	100	100
9	W	202/204 (99%)	193 (96%)	9 (4%)	0	100	100
10	J	196/198 (99%)	184 (94%)	11 (6%)	1 (0%)	31	56
10	X	196/198 (99%)	184 (94%)	11 (6%)	1 (0%)	31	56
11	K	210/212 (99%)	202 (96%)	7 (3%)	1 (0%)	31	56
11	Y	210/212 (99%)	202 (96%)	7 (3%)	1 (0%)	31	56
12	L	220/222 (99%)	209 (95%)	10 (4%)	1 (0%)	31	56
12	Z	220/222 (99%)	208 (94%)	11 (5%)	1 (0%)	31	56
13	1	231/233 (99%)	217 (94%)	14 (6%)	0	100	100
13	M	231/233 (99%)	217 (94%)	14 (6%)	0	100	100
14	2	194/196 (99%)	188 (97%)	6 (3%)	0	100	100
14	N	194/196 (99%)	188 (97%)	6 (3%)	0	100	100
All	All	6312/6368 (99%)	5948 (94%)	310 (5%)	54 (1%)	19	38

5 of 54 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	5	THR

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Mol	Chain	Res	Type
1	A	56	SER
3	C	58	LEU
4	D	12(G)	GLU
10	J	192	ALA

### 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	209/209 (100%)	204 (98%)	5 (2%)	52	77
1	O	209/209 (100%)	204 (98%)	5 (2%)	52	77
2	B	203/203 (100%)	195 (96%)	8 (4%)	35	62
2	P	203/203 (100%)	195 (96%)	8 (4%)	35	62
3	C	213/213 (100%)	204 (96%)	9 (4%)	32	59
3	Q	213/213 (100%)	204 (96%)	9 (4%)	32	59
4	D	198/198 (100%)	187 (94%)	11 (6%)	23	45
4	R	198/198 (100%)	187 (94%)	11 (6%)	23	45
5	E	192/192 (100%)	171 (89%)	21 (11%)	7	12
5	S	192/192 (100%)	171 (89%)	21 (11%)	7	12
6	F	201/201 (100%)	186 (92%)	15 (8%)	15	29
6	T	201/201 (100%)	185 (92%)	16 (8%)	13	26
7	G	207/207 (100%)	193 (93%)	14 (7%)	17	35
7	U	207/207 (100%)	192 (93%)	15 (7%)	16	32
8	H	181/181 (100%)	173 (96%)	8 (4%)	31	57
8	V	181/181 (100%)	174 (96%)	7 (4%)	35	62
9	I	172/172 (100%)	168 (98%)	4 (2%)	53	78
9	W	172/172 (100%)	168 (98%)	4 (2%)	53	78
10	J	175/175 (100%)	168 (96%)	7 (4%)	34	61
10	X	175/175 (100%)	168 (96%)	7 (4%)	34	61

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	K	169/169 (100%)	162 (96%)	7 (4%)	33	60
11	Y	169/169 (100%)	161 (95%)	8 (5%)	29	54
12	L	185/185 (100%)	174 (94%)	11 (6%)	21	43
12	Z	185/185 (100%)	173 (94%)	12 (6%)	19	38
13	1	199/199 (100%)	189 (95%)	10 (5%)	27	51
13	M	199/199 (100%)	190 (96%)	9 (4%)	30	56
14	2	162/162 (100%)	152 (94%)	10 (6%)	20	40
14	N	162/162 (100%)	152 (94%)	10 (6%)	20	40
All	All	5332/5332 (100%)	5050 (95%)	282 (5%)	25	48

5 of 282 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
13	M	204	LYS
3	Q	150	GLN
12	Z	1(I)	ASN
14	N	89	GLU
1	O	179	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 194 such sidechains are listed below:

Mol	Chain	Res	Type
13	M	89	GLN
3	Q	121	GLN
12	Z	1(I)	ASN
13	M	157	ASN
2	P	23	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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

6 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
15	FEB	2	0	14	38,38,38	1.50	6 (15%)	46,47,47	1.19	4 (8%)
15	FEB	H	0	8	38,38,38	0.82	0	46,47,47	0.88	1 (2%)
15	FEB	K	0	11	38,38,38	0.88	1 (2%)	46,47,47	0.78	0
15	FEB	N	0	14	38,38,38	1.47	5 (13%)	46,47,47	1.15	5 (10%)
15	FEB	V	0	8	38,38,38	0.80	0	46,47,47	0.90	0
15	FEB	Y	0	11	38,38,38	0.88	1 (2%)	46,47,47	0.76	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	FEB	2	0	14	-	0/48/48/48	0/0/0/0
15	FEB	H	0	8	-	0/48/48/48	0/0/0/0
15	FEB	K	0	11	-	0/48/48/48	0/0/0/0
15	FEB	N	0	14	-	0/48/48/48	0/0/0/0
15	FEB	V	0	8	-	0/48/48/48	0/0/0/0
15	FEB	Y	0	11	-	0/48/48/48	0/0/0/0

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	2	0	FEB	C29-C26	2.02	1.61	1.52
15	N	0	FEB	C3-C2	2.05	1.55	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	N	0	FEB	C10-C11	2.07	1.58	1.52
15	Y	0	FEB	C19-N18	2.13	1.50	1.45
15	N	0	FEB	O21-C20	2.25	1.27	1.23

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	N	0	FEB	C19-C20-N9	-2.13	112.06	116.77
15	H	0	FEB	C19-C22-C23	2.14	116.58	112.27
15	N	0	FEB	C20-C19-N18	2.34	117.55	111.18
15	2	0	FEB	C20-C19-N18	2.53	118.09	111.18
15	N	0	FEB	C10-N9-C20	2.60	127.27	121.66

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	2	0	FEB	6	0
15	H	0	FEB	3	0
15	N	0	FEB	7	0
15	V	0	FEB	3	0

## 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	250/250 (100%)	-0.09	9 (3%)	42	35	34, 52, 85, 106	0
1	O	250/250 (100%)	-0.01	14 (5%)	24	18	35, 54, 85, 105	0
2	B	244/244 (100%)	0.18	14 (5%)	24	17	37, 56, 89, 116	0
2	P	244/244 (100%)	0.19	15 (6%)	21	15	40, 56, 89, 116	0
3	C	241/241 (100%)	0.41	26 (10%)	6	3	39, 61, 110, 124	0
3	Q	241/241 (100%)	0.54	37 (15%)	2	1	41, 62, 110, 124	0
4	D	242/242 (100%)	0.22	17 (7%)	16	11	43, 58, 94, 121	0
4	R	242/242 (100%)	0.29	17 (7%)	16	11	44, 59, 95, 122	0
5	E	233/233 (100%)	0.02	9 (3%)	39	31	42, 55, 82, 109	0
5	S	233/233 (100%)	-0.03	8 (3%)	45	37	41, 54, 82, 109	0
6	F	244/244 (100%)	-0.17	9 (3%)	41	33	36, 50, 89, 106	0
6	T	244/244 (100%)	-0.18	7 (2%)	51	44	34, 50, 89, 106	0
7	G	243/243 (100%)	-0.18	9 (3%)	41	33	33, 47, 75, 112	0
7	U	243/243 (100%)	-0.12	8 (3%)	46	39	33, 47, 75, 111	0
8	H	222/222 (100%)	-0.36	3 (1%)	75	71	30, 44, 62, 100	0
8	V	222/222 (100%)	-0.41	3 (1%)	75	71	29, 45, 63, 100	0
9	I	204/204 (100%)	-0.37	4 (1%)	65	59	35, 45, 63, 80	0
9	W	204/204 (100%)	-0.35	3 (1%)	73	69	36, 46, 64, 80	0
10	J	198/198 (100%)	-0.09	8 (4%)	38	30	38, 49, 69, 122	0
10	X	198/198 (100%)	-0.10	6 (3%)	50	43	38, 49, 69, 122	0
11	K	212/212 (100%)	-0.12	10 (4%)	31	25	34, 47, 72, 86	0
11	Y	212/212 (100%)	-0.15	11 (5%)	27	20	35, 47, 74, 86	0
12	L	222/222 (100%)	-0.18	6 (2%)	54	48	33, 48, 74, 89	0
12	Z	222/222 (100%)	-0.23	10 (4%)	33	26	34, 47, 74, 89	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	1	233/233 (100%)	-0.47	1 (0%) 92 91	31, 43, 57, 61	0
13	M	233/233 (100%)	-0.40	2 (0%) 84 81	32, 43, 57, 63	0
14	2	196/196 (100%)	-0.40	2 (1%) 82 79	31, 41, 61, 81	0
14	N	196/196 (100%)	-0.40	1 (0%) 90 89	31, 40, 60, 81	0
All	All	6368/6368 (100%)	-0.10	269 (4%) 36 28	29, 50, 84, 124	0

The worst 5 of 269 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	D	12(C)	GLY	13.2
3	C	55	THR	12.6
4	R	12(E)	SER	11.7
4	D	12(E)	SER	10.0
10	X	192	ALA	9.8

## 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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
15	FEB	2	0	39/39	0.88	0.27	39,50,60,65	0
15	FEB	N	0	39/39	0.90	0.22	40,49,60,61	0
15	FEB	V	0	39/39	0.91	0.20	39,45,58,63	0
15	FEB	Y	0	39/39	0.91	0.20	34,43,56,58	0
15	FEB	K	0	39/39	0.92	0.18	32,40,55,56	0
15	FEB	H	0	39/39	0.93	0.17	38,45,58,63	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.