



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 07:15 am GMT

PDB ID : 4LQI  
Title : Yeast 20S Proteasome in complex with Vibralactone  
Authors : List, A.; Zeiler, E.; Gallastegui, N.; Rusch, M.; Hedberg, C.; Sieber, S.A.; Groll, M.  
Deposited on : 2013-07-18  
Resolution : 2.70 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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : recalc28949

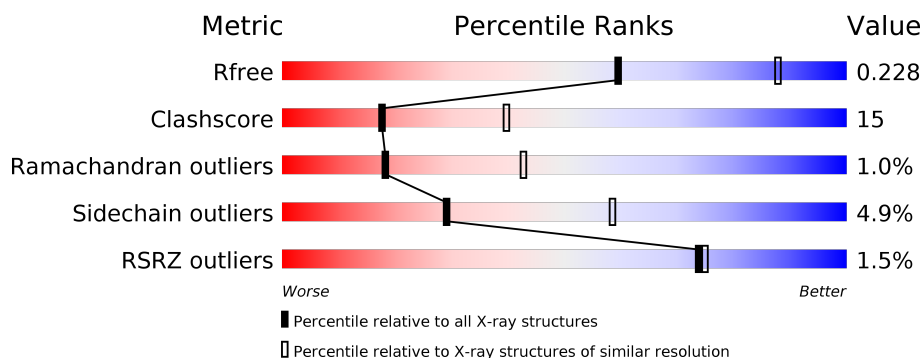
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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.



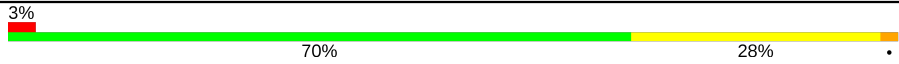



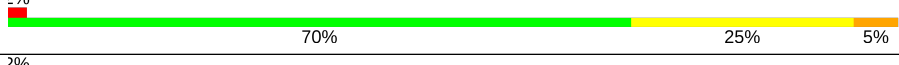
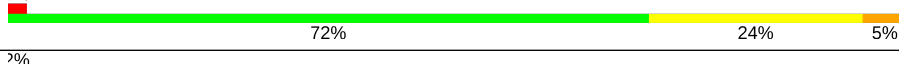
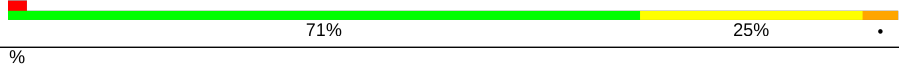

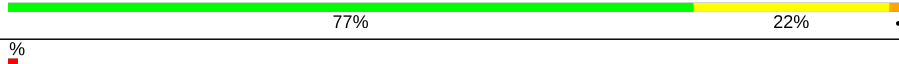


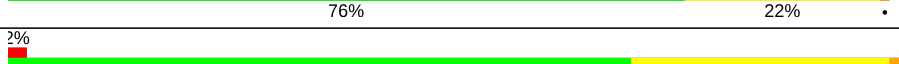

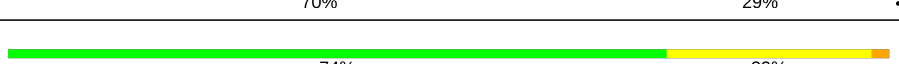

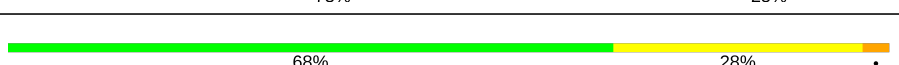
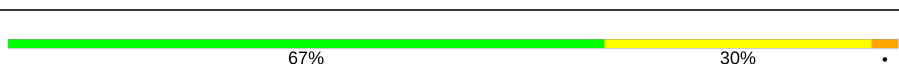
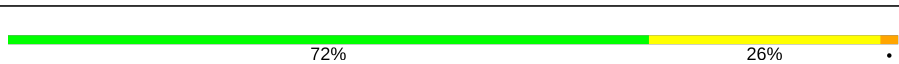
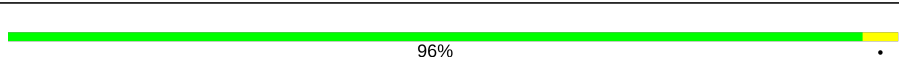

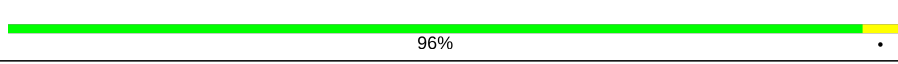
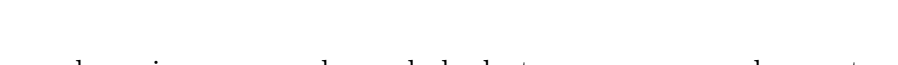
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	100719	2259 (2.70-2.70)
Clashscore	112137	2590 (2.70-2.70)
Ramachandran outliers	110173	2550 (2.70-2.70)
Sidechain outliers	110143	2550 (2.70-2.70)
RSRZ outliers	101464	2275 (2.70-2.70)

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>0%</div> <div> <div></div> <div>76%</div> <div>23%</div> <div>•</div> </div> </div>
1	O	250	<div> <div>2%</div> <div> <div></div> <div>74%</div> <div>25%</div> <div>•</div> </div> </div>
2	B	244	<div> <div>2%</div> <div> <div></div> <div>64%</div> <div>31%</div> <div>5%</div> </div> </div>
2	P	244	<div> <div>3%</div> <div> <div></div> <div>66%</div> <div>30%</div> <div>5%</div> </div> </div>
3	C	241	<div> <div>2%</div> <div> <div></div> <div>60%</div> <div>37%</div> <div>•</div> </div> </div>
3	Q	241	<div> <div>7%</div> <div> <div></div> <div>60%</div> <div>37%</div> <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	M	233	
13	a	233	
14	N	196	
14	b	196	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
15	1Y9	K	301	-	-	-	X
15	1Y9	N	201	-	-	-	X
15	1Y9	Y	301	-	-	-	X
15	1Y9	b	201	-	-	-	X

## 2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 50942 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 subunit alpha type-2.

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 subunit alpha type-3.

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 subunit alpha type-4.

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			

- Molecule 4 is a protein called Proteasome subunit alpha type-5.

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 subunit alpha type-6.

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 subunit alpha type-7.

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 subunit alpha type-1.

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			

- Molecule 8 is a protein called Proteasome subunit beta type-2.

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 subunit beta type-3.

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 subunit beta type-4.

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

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

- Molecule 11 is a protein called Proteasome subunit beta type-5.

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 subunit beta type-6.

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

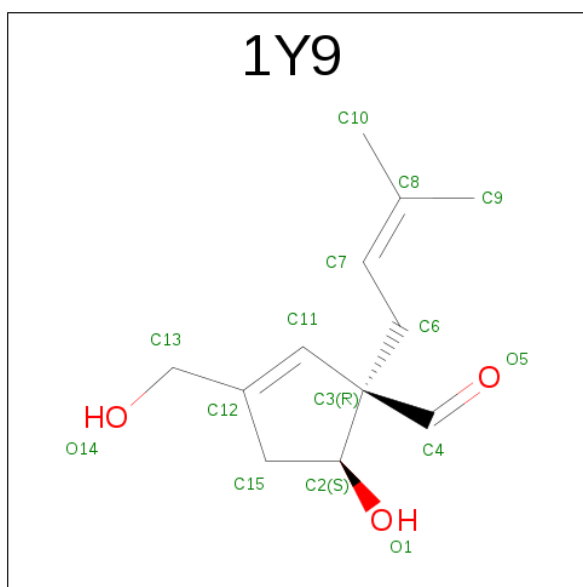
- Molecule 13 is a protein called Proteasome subunit beta type-7.

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

- Molecule 14 is a protein called Proteasome subunit beta type-1.

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

- Molecule 15 is VIBRALACTONE, BOUND FORM (three-letter code: 1Y9) (formula: C<sub>12</sub>H<sub>18</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
15	K	1	Total	C	O	0	0
			15	12	3		
15	N	1	Total	C	O	0	0
			15	12	3		
15	Y	1	Total	C	O	0	0
			15	12	3		
15	b	1	Total	C	O	0	0
			15	12	3		

- Molecule 16 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	A	56	Total	O	0	0
			56	56		
16	B	36	Total	O	0	0
			36	36		
16	C	42	Total	O	0	0
			42	42		
16	D	38	Total	O	0	0
			38	38		
16	E	23	Total	O	0	0
			23	23		
16	F	49	Total	O	0	0
			49	49		
16	G	61	Total	O	0	0
			61	61		
16	H	49	Total	O	0	0
			49	49		

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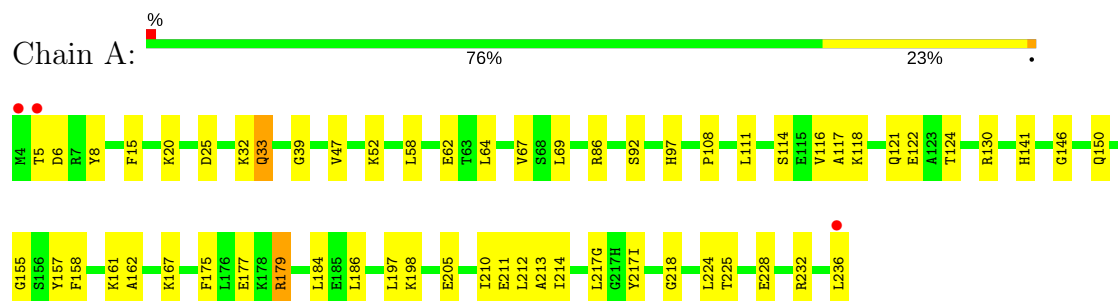
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	I	70	Total 70	O 70	0	0
16	J	53	Total 53	O 53	0	0
16	K	46	Total 46	O 46	0	0
16	L	56	Total 56	O 56	0	0
16	M	73	Total 73	O 73	0	0
16	N	57	Total 57	O 57	0	0
16	O	31	Total 31	O 31	0	0
16	P	28	Total 28	O 28	0	0
16	Q	28	Total 28	O 28	0	0
16	R	31	Total 31	O 31	0	0
16	S	20	Total 20	O 20	0	0
16	T	38	Total 38	O 38	0	0
16	U	62	Total 62	O 62	0	0
16	V	46	Total 46	O 46	0	0
16	W	61	Total 61	O 61	0	0
16	X	52	Total 52	O 52	0	0
16	Y	46	Total 46	O 46	0	0
16	Z	52	Total 52	O 52	0	0
16	a	75	Total 75	O 75	0	0
16	b	55	Total 55	O 55	0	0

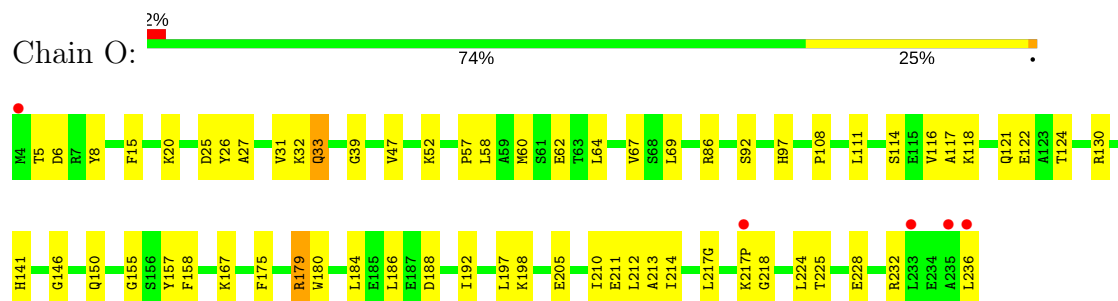
### 3 Residue-property plots [i](#)

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.

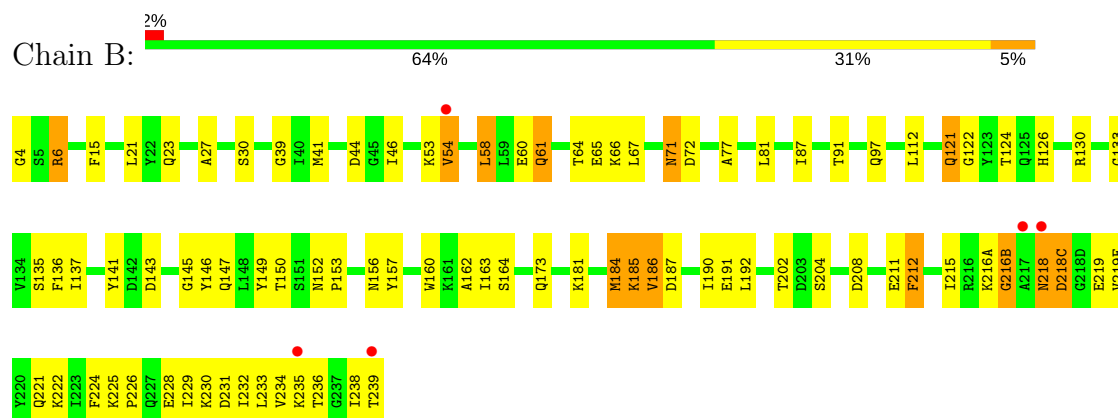
#### • Molecule 1: Proteasome subunit alpha type-2



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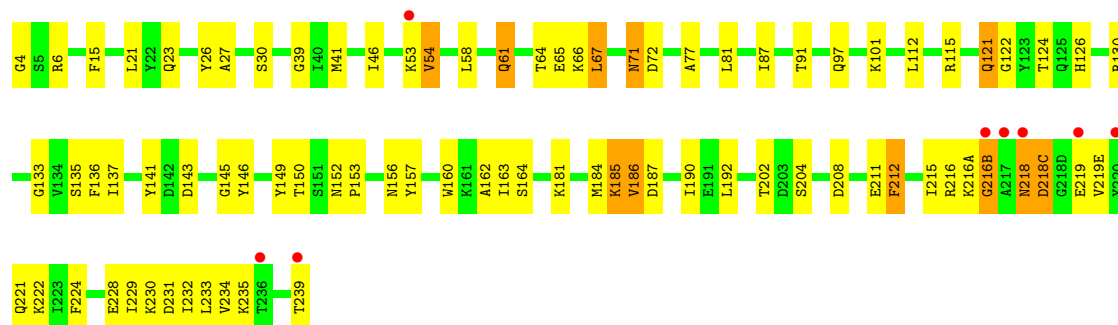


#### • Molecule 2: Proteasome subunit alpha type-3

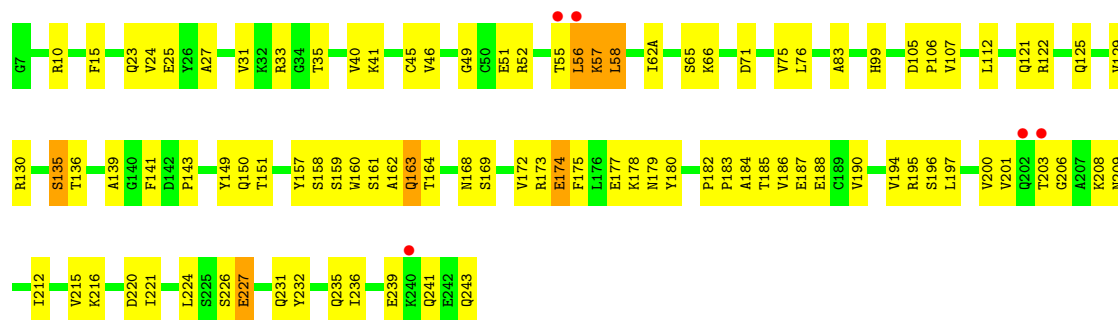


#### • Molecule 2: Proteasome subunit alpha type-3

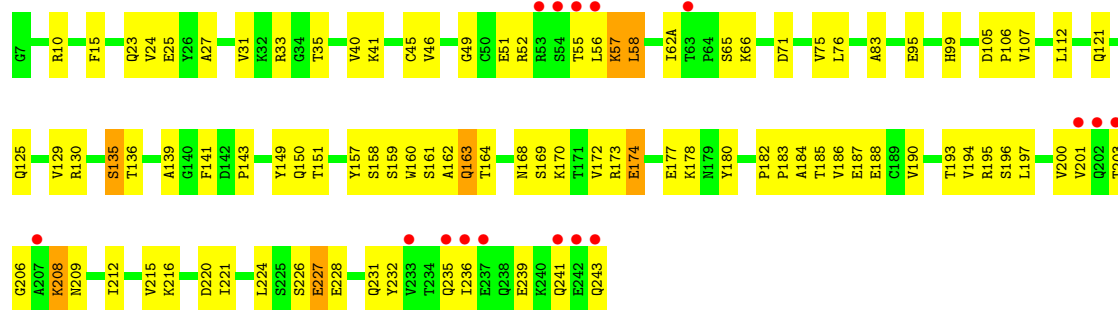




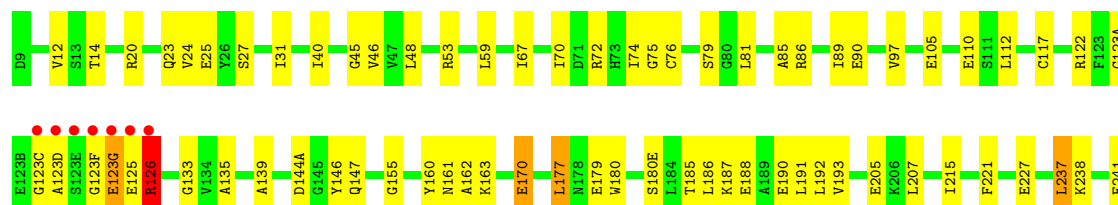
• Molecule 3: Proteasome subunit alpha type-4



• Molecule 3: Proteasome subunit alpha type-4

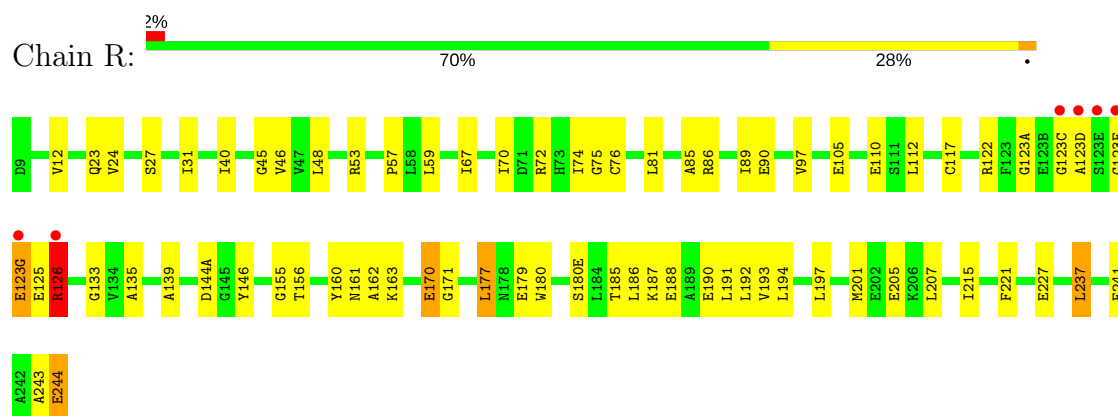


• Molecule 4: Proteasome subunit alpha type-5

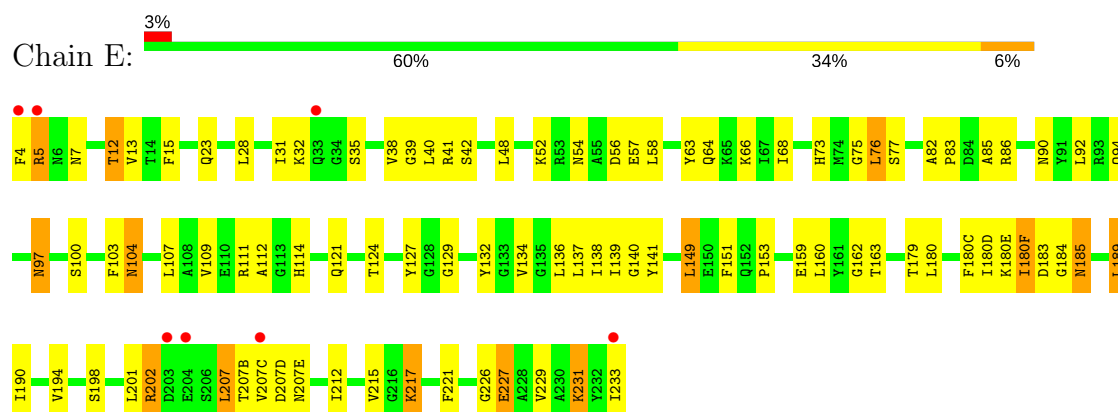




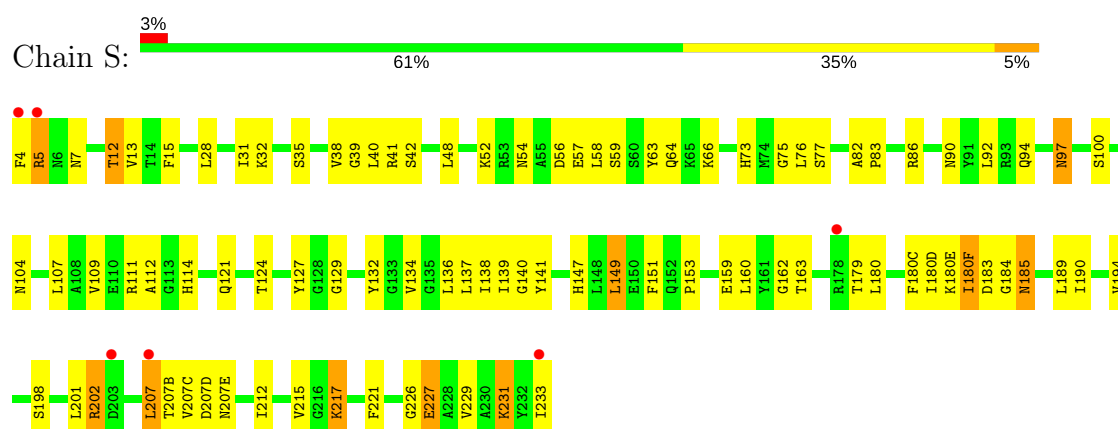
• Molecule 4: Proteasome subunit alpha type-5



• Molecule 5: Proteasome subunit alpha type-6

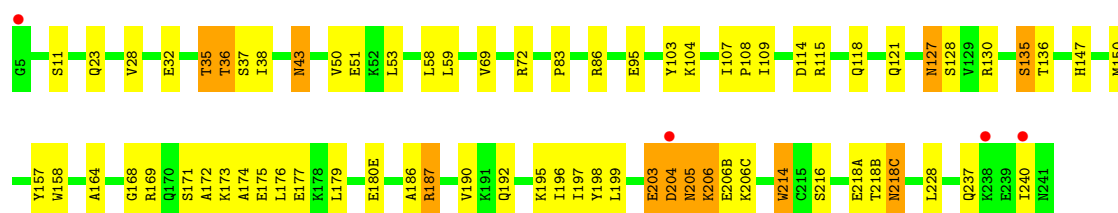


• Molecule 5: Proteasome subunit alpha type-6

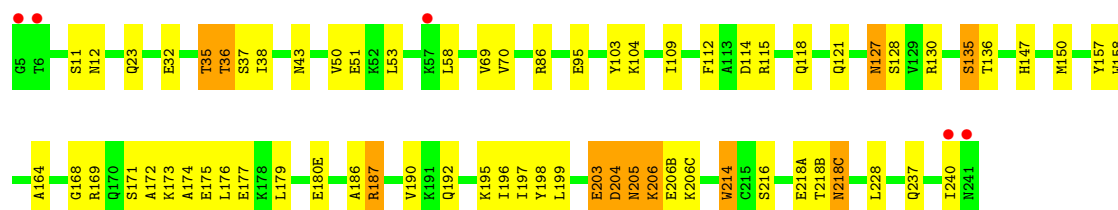


• Molecule 6: Proteasome subunit alpha type-7

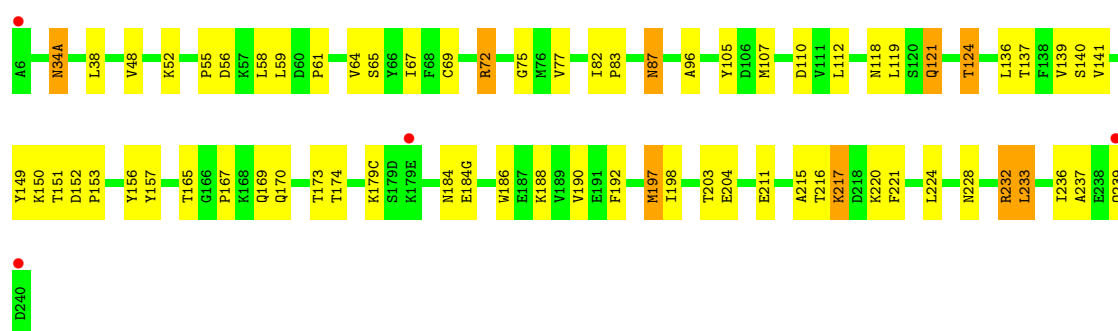




• Molecule 6: Proteasome subunit alpha type-7



• Molecule 7: Proteasome subunit alpha type-1



• Molecule 7: Proteasome subunit alpha type-1

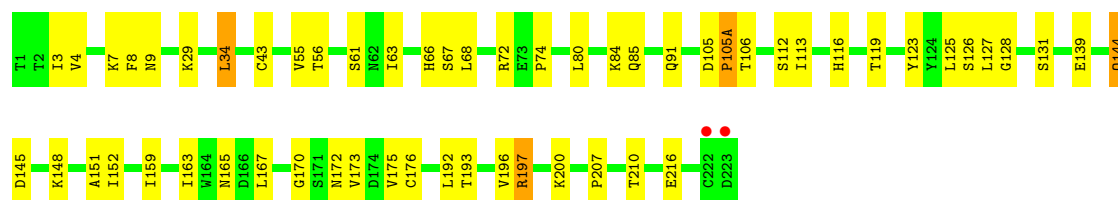
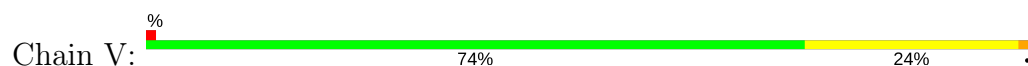


• Molecule 8: Proteasome subunit beta type-2

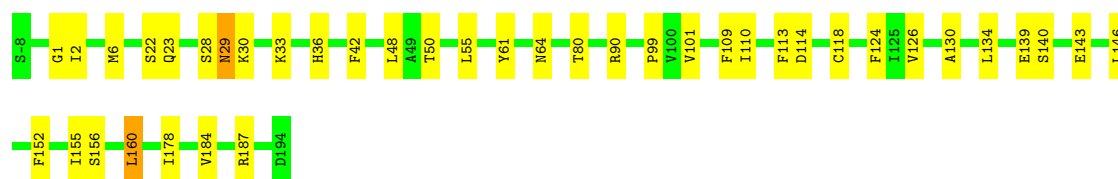




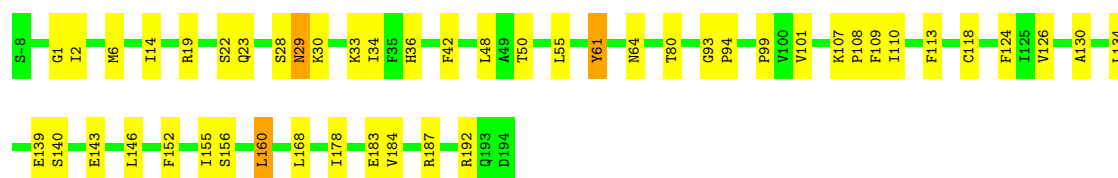
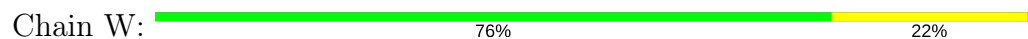
• Molecule 8: Proteasome subunit beta type-2



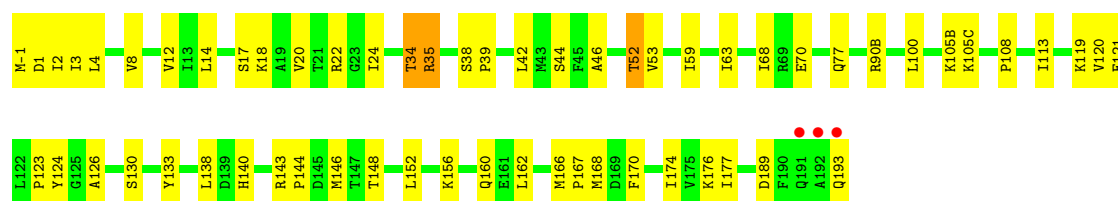
• Molecule 9: Proteasome subunit beta type-3



• Molecule 9: Proteasome subunit beta type-3

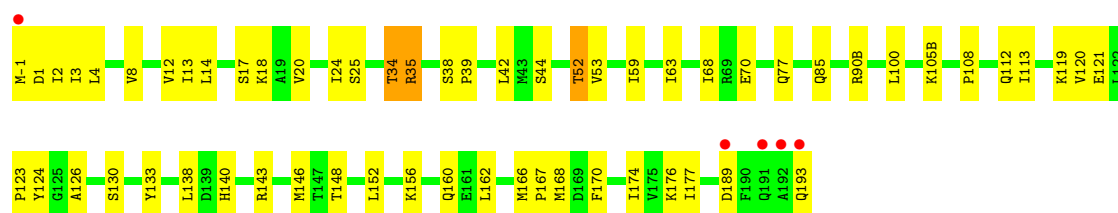


• Molecule 10: Proteasome subunit beta type-4



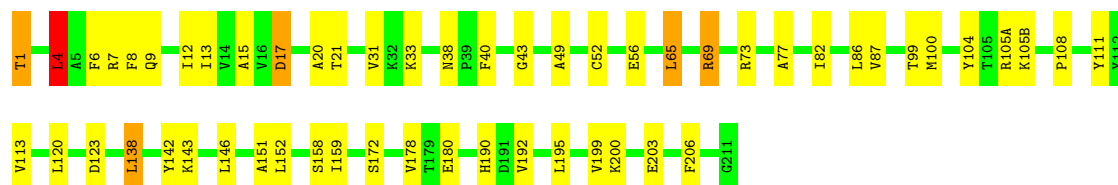
• Molecule 10: Proteasome subunit beta type-4





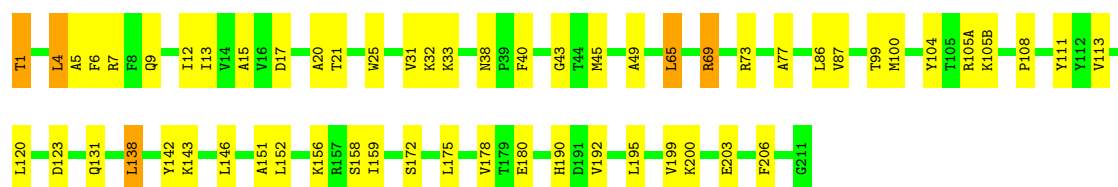
• Molecule 11: Proteasome subunit beta type-5

Chain K: 74% 23%



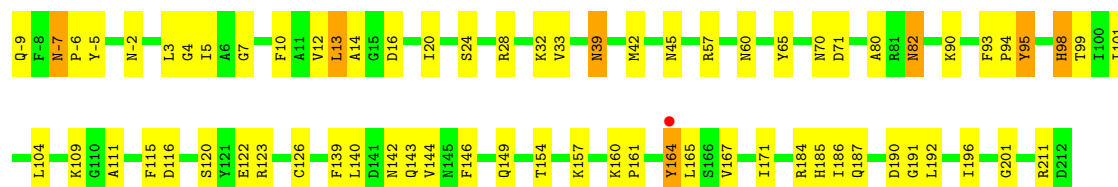
• Molecule 11: Proteasome subunit beta type-5

Chain Y: 73% 25%



• Molecule 12: Proteasome subunit beta type-6

Chain L: 68% 28%

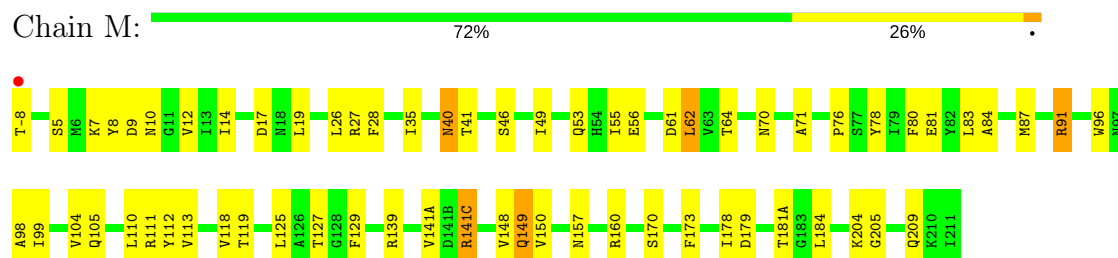


• Molecule 12: Proteasome subunit beta type-6

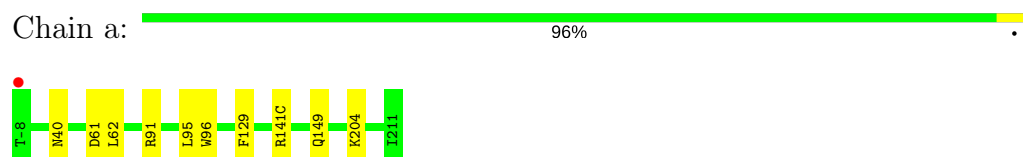
Chain Z: 67% 30%



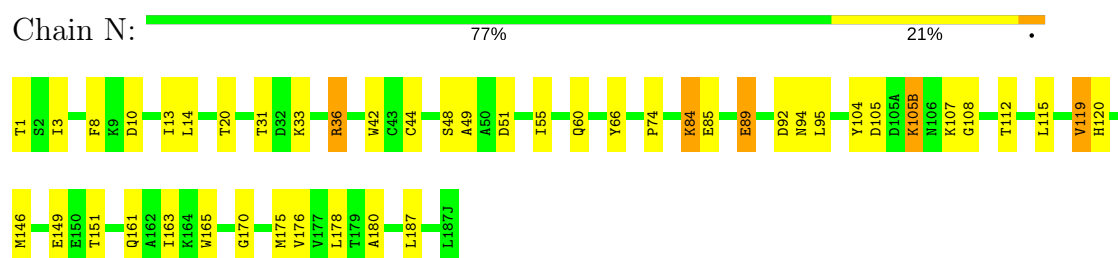
- Molecule 13: Proteasome subunit beta type-7



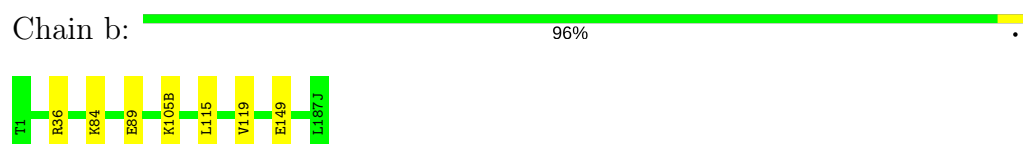
- Molecule 13: Proteasome subunit beta type-7



- Molecule 14: Proteasome subunit beta type-1



- Molecule 14: Proteasome subunit beta type-1





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	135.86Å 299.40Å 144.99Å 90.00° 113.07° 90.00°	Depositor
Resolution (Å)	14.99 – 2.70 48.95 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.4 (14.99-2.70) 99.5 (48.95-2.70)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.97 (at 2.69Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, $R_{free}$	0.202 , 0.227 0.202 , 0.228	Depositor DCC
$R_{free}$ test set	14275 reflections (4.97%)	DCC
Wilson B-factor (Å <sup>2</sup> )	53.8	Xtriage
Anisotropy	0.619	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 49.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	50942	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.08% 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 ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 1Y9

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	0.37	0/1952	0.63	0/2642
1	O	0.38	0/1952	0.63	0/2642
2	B	0.38	0/1935	0.62	0/2618
2	P	0.39	0/1935	0.62	0/2618
3	C	0.36	0/1920	0.62	1/2598 (0.0%)
3	Q	0.36	0/1920	0.62	0/2598
4	D	0.35	0/1887	0.62	0/2541
4	R	0.37	0/1887	0.62	0/2541
5	E	0.36	0/1823	0.60	0/2463
5	S	0.36	0/1823	0.60	0/2463
6	F	0.38	0/1937	0.62	1/2614 (0.0%)
6	T	0.38	0/1937	0.62	1/2614 (0.0%)
7	G	0.40	0/1959	0.62	0/2652
7	U	0.40	0/1959	0.62	0/2652
8	H	0.40	0/1716	0.66	0/2326
8	V	0.39	0/1716	0.66	0/2326
9	I	0.40	0/1611	0.66	0/2174
9	W	0.40	0/1611	0.67	0/2174
10	J	0.40	0/1613	0.64	0/2173
10	X	0.40	0/1613	0.65	0/2173
11	K	0.41	0/1681	0.65	1/2274 (0.0%)
11	Y	0.41	0/1681	0.65	0/2274
12	L	0.40	0/1795	0.66	1/2420 (0.0%)
12	Z	0.40	0/1795	0.66	1/2420 (0.0%)
13	M	0.39	0/1855	0.66	0/2514
13	a	0.39	0/1855	0.66	1/2514 (0.0%)
14	N	0.40	0/1541	0.63	0/2087
14	b	0.39	0/1541	0.62	0/2087
All	All	0.39	0/50450	0.64	7/68192 (0.0%)

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(°)
12	L	95	TYR	N-CA-C	-5.26	96.80	111.00
12	Z	95	TYR	N-CA-C	-5.23	96.89	111.00
6	T	135	SER	N-CA-C	-5.21	96.94	111.00
6	F	135	SER	N-CA-C	-5.20	96.96	111.00
13	a	95	LEU	N-CA-C	-5.18	97.02	111.00

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	1915	0	1926	54	0
1	O	1915	0	1926	58	0
2	B	1905	0	1901	80	0
2	P	1905	0	1901	75	0
3	C	1891	0	1900	95	0
3	Q	1891	0	1900	99	0
4	D	1862	0	1836	51	0
4	R	1862	0	1836	53	0
5	E	1795	0	1797	88	0
5	S	1795	0	1797	85	0
6	F	1897	0	1886	62	0
6	T	1897	0	1886	61	0
7	G	1921	0	1910	66	0
7	U	1921	0	1910	74	0
8	H	1685	0	1688	40	0
8	V	1685	0	1688	42	0
9	I	1581	0	1574	36	0
9	W	1581	0	1574	39	0
10	J	1585	0	1590	64	0
10	X	1585	0	1590	68	0
11	K	1644	0	1594	49	0
11	Y	1644	0	1594	51	0
12	L	1757	0	1711	52	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	Z	1757	0	1711	54	0
13	M	1824	0	1832	52	0
13	a	1824	0	1832	0	0
14	N	1512	0	1480	36	0
14	b	1512	0	1480	0	0
15	K	15	0	17	2	0
15	N	15	0	17	3	0
15	Y	15	0	17	2	0
15	b	15	0	17	0	0
16	A	56	0	0	0	0
16	B	36	0	0	2	0
16	C	42	0	0	2	0
16	D	38	0	0	2	0
16	E	23	0	0	0	0
16	F	49	0	0	2	0
16	G	61	0	0	3	0
16	H	49	0	0	4	0
16	I	70	0	0	3	0
16	J	53	0	0	3	0
16	K	46	0	0	2	0
16	L	56	0	0	1	0
16	M	73	0	0	1	0
16	N	57	0	0	4	0
16	O	31	0	0	2	0
16	P	28	0	0	2	0
16	Q	28	0	0	4	0
16	R	31	0	0	1	0
16	S	20	0	0	0	0
16	T	38	0	0	3	0
16	U	62	0	0	3	0
16	V	46	0	0	3	0
16	W	61	0	0	2	0
16	X	52	0	0	3	0
16	Y	46	0	0	1	0
16	Z	52	0	0	3	0
16	a	75	0	0	0	0
16	b	55	0	0	0	0
All	All	50942	0	49318	1418	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 15.

The worst 5 of 1418 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)
2:P:202:THR:HG22	2:P:204:SER:H	1.13	1.09
2:B:202:THR:HG22	2:B:204:SER:H	1.14	1.07
7:G:96:ALA:HA	7:G:107:MET:HE2	1.40	1.03
7:U:96:ALA:HA	7:U:107:MET:HE2	1.43	1.00
11:K:105(B):LYS:HD2	11:K:105(B):LYS:H	1.26	1.00

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%)	235 (95%)	11 (4%)	2 (1%)	22	49
1	O	248/250 (99%)	235 (95%)	11 (4%)	2 (1%)	22	49
2	B	242/244 (99%)	219 (90%)	16 (7%)	7 (3%)	5	13
2	P	242/244 (99%)	219 (90%)	17 (7%)	6 (2%)	6	17
3	C	239/241 (99%)	226 (95%)	10 (4%)	3 (1%)	14	35
3	Q	239/241 (99%)	225 (94%)	11 (5%)	3 (1%)	14	35
4	D	240/242 (99%)	223 (93%)	13 (5%)	4 (2%)	11	27
4	R	240/242 (99%)	221 (92%)	15 (6%)	4 (2%)	11	27
5	E	231/233 (99%)	208 (90%)	16 (7%)	7 (3%)	5	12
5	S	231/233 (99%)	208 (90%)	16 (7%)	7 (3%)	5	12
6	F	242/244 (99%)	231 (96%)	9 (4%)	2 (1%)	22	49
6	T	242/244 (99%)	231 (96%)	9 (4%)	2 (1%)	22	49
7	G	241/243 (99%)	227 (94%)	13 (5%)	1 (0%)	38	66
7	U	241/243 (99%)	227 (94%)	13 (5%)	1 (0%)	38	66
8	H	220/222 (99%)	209 (95%)	9 (4%)	2 (1%)	20	46
8	V	220/222 (99%)	209 (95%)	8 (4%)	3 (1%)	13	33

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	I	202/204 (99%)	193 (96%)	9 (4%)	0	100	100
9	W	202/204 (99%)	193 (96%)	9 (4%)	0	100	100
10	J	196/198 (99%)	186 (95%)	9 (5%)	1 (0%)	32	60
10	X	196/198 (99%)	187 (95%)	8 (4%)	1 (0%)	32	60
11	K	210/212 (99%)	202 (96%)	8 (4%)	0	100	100
11	Y	210/212 (99%)	203 (97%)	7 (3%)	0	100	100
12	L	220/222 (99%)	206 (94%)	13 (6%)	1 (0%)	32	60
12	Z	220/222 (99%)	207 (94%)	12 (6%)	1 (0%)	32	60
13	M	231/233 (99%)	219 (95%)	11 (5%)	1 (0%)	38	66
13	a	231/233 (99%)	219 (95%)	11 (5%)	1 (0%)	38	66
14	N	194/196 (99%)	189 (97%)	5 (3%)	0	100	100
14	b	194/196 (99%)	189 (97%)	5 (3%)	0	100	100
All	All	6312/6368 (99%)	5946 (94%)	304 (5%)	62 (1%)	18	43

5 of 62 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	54	VAL
2	B	218(C)	ASP
3	C	58	LEU
3	C	203	THR
4	D	123(G)	GLU

### 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%)	205 (98%)	4 (2%)	62	87
1	O	209/209 (100%)	205 (98%)	4 (2%)	62	87
2	B	203/203 (100%)	193 (95%)	10 (5%)	29	58
2	P	203/203 (100%)	192 (95%)	11 (5%)	26	54

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C	213/213 (100%)	203 (95%)	10 (5%)	30	60
3	Q	213/213 (100%)	203 (95%)	10 (5%)	30	60
4	D	198/198 (100%)	186 (94%)	12 (6%)	22	47
4	R	198/198 (100%)	186 (94%)	12 (6%)	22	47
5	E	192/192 (100%)	176 (92%)	16 (8%)	13	30
5	S	192/192 (100%)	177 (92%)	15 (8%)	15	33
6	F	201/201 (100%)	186 (92%)	15 (8%)	16	36
6	T	201/201 (100%)	186 (92%)	15 (8%)	16	36
7	G	207/207 (100%)	195 (94%)	12 (6%)	23	50
7	U	207/207 (100%)	195 (94%)	12 (6%)	23	50
8	H	181/181 (100%)	174 (96%)	7 (4%)	37	68
8	V	181/181 (100%)	174 (96%)	7 (4%)	37	68
9	I	172/172 (100%)	169 (98%)	3 (2%)	66	88
9	W	172/172 (100%)	169 (98%)	3 (2%)	66	88
10	J	175/175 (100%)	169 (97%)	6 (3%)	42	73
10	X	175/175 (100%)	169 (97%)	6 (3%)	42	73
11	K	169/169 (100%)	159 (94%)	10 (6%)	23	49
11	Y	169/169 (100%)	160 (95%)	9 (5%)	26	54
12	L	185/185 (100%)	174 (94%)	11 (6%)	23	49
12	Z	185/185 (100%)	173 (94%)	12 (6%)	20	44
13	M	199/199 (100%)	191 (96%)	8 (4%)	36	67
13	a	199/199 (100%)	191 (96%)	8 (4%)	36	67
14	N	162/162 (100%)	155 (96%)	7 (4%)	33	64
14	b	162/162 (100%)	155 (96%)	7 (4%)	33	64
All	All	5332/5332 (100%)	5070 (95%)	262 (5%)	29	58

5 of 262 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
13	M	62	LEU
3	Q	10	ARG
12	Z	98	HIS
13	M	149	GLN
1	O	158	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 201 such sidechains are listed below:

Mol	Chain	Res	Type
13	M	93	ASN
3	Q	82	ASN
12	Z	155	ASN
13	M	172	ASN
1	O	97	HIS

### 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](#)

4 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	1Y9	K	301	11	12,15,15	2.25	2 (16%)	11,21,21	1.89	3 (27%)
15	1Y9	N	201	14	12,15,15	2.14	1 (8%)	11,21,21	2.14	2 (18%)
15	1Y9	Y	301	11	12,15,15	2.21	2 (16%)	11,21,21	1.81	3 (27%)
15	1Y9	b	201	14	12,15,15	2.15	1 (8%)	11,21,21	2.03	2 (18%)

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	1Y9	K	301	11	-	0/10/26/26	0/1/1/1
15	1Y9	N	201	14	-	0/10/26/26	0/1/1/1
15	1Y9	Y	301	11	-	0/10/26/26	0/1/1/1
15	1Y9	b	201	14	-	0/10/26/26	0/1/1/1

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	K	301	1Y9	C15-C2	2.04	1.55	1.53
15	Y	301	1Y9	C15-C2	2.67	1.55	1.53
15	Y	301	1Y9	O5-C4	6.71	1.43	1.19
15	b	201	1Y9	O5-C4	6.75	1.43	1.19
15	N	201	1Y9	O5-C4	6.84	1.44	1.19

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	b	201	1Y9	C6-C3-C4	-3.34	102.99	108.14
15	N	201	1Y9	C6-C3-C4	-3.30	103.04	108.14
15	Y	301	1Y9	C6-C3-C4	-3.17	103.24	108.14
15	K	301	1Y9	C6-C3-C4	-3.15	103.28	108.14
15	Y	301	1Y9	C15-C12-C11	2.02	113.78	110.89

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	K	301	1Y9	2	0
15	N	201	1Y9	3	0
15	Y	301	1Y9	2	0

## 5.7 Other polymers ⓘ

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	250/250 (100%)	-0.26	3 (1%) 79 80	44, 58, 89, 114	0
1	O	250/250 (100%)	-0.22	5 (2%) 65 66	44, 59, 91, 114	0
2	B	244/244 (100%)	-0.15	5 (2%) 65 66	42, 62, 102, 124	0
2	P	244/244 (100%)	-0.06	8 (3%) 47 46	42, 63, 103, 124	0
3	C	241/241 (100%)	-0.07	5 (2%) 64 65	45, 67, 117, 132	0
3	Q	241/241 (100%)	0.13	16 (6%) 19 17	47, 69, 118, 133	0
4	D	242/242 (100%)	-0.02	7 (2%) 52 52	45, 66, 98, 133	0
4	R	242/242 (100%)	-0.10	6 (2%) 58 58	46, 67, 97, 133	0
5	E	233/233 (100%)	0.00	7 (3%) 51 50	49, 69, 95, 121	0
5	S	233/233 (100%)	-0.02	6 (2%) 56 56	49, 70, 95, 120	0
6	F	244/244 (100%)	-0.25	4 (1%) 72 73	45, 62, 99, 114	0
6	T	244/244 (100%)	-0.07	5 (2%) 65 66	46, 63, 99, 115	0
7	G	243/243 (100%)	-0.32	4 (1%) 72 73	40, 57, 87, 123	0
7	U	243/243 (100%)	-0.34	3 (1%) 79 80	39, 57, 86, 124	0
8	H	222/222 (100%)	-0.33	0 100 100	41, 55, 77, 108	0
8	V	222/222 (100%)	-0.40	2 (0%) 84 85	42, 56, 78, 110	0
9	I	204/204 (100%)	-0.40	0 100 100	39, 53, 71, 84	0
9	W	204/204 (100%)	-0.31	0 100 100	40, 53, 72, 85	0
10	J	198/198 (100%)	-0.33	3 (1%) 74 75	42, 55, 74, 133	0
10	X	198/198 (100%)	-0.32	5 (2%) 58 58	43, 56, 73, 133	0
11	K	212/212 (100%)	-0.41	0 100 100	39, 54, 73, 83	0
11	Y	212/212 (100%)	-0.44	0 100 100	40, 54, 74, 84	0
12	L	222/222 (100%)	-0.41	1 (0%) 90 92	38, 55, 78, 97	0
12	Z	222/222 (100%)	-0.36	1 (0%) 90 92	39, 55, 76, 97	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	M	233/233 (100%)	-0.44	1 (0%) 92 93	39, 56, 71, 79	0
13	a	233/233 (100%)	-0.48	1 (0%) 92 93	39, 55, 71, 79	0
14	N	196/196 (100%)	-0.49	0 100 100	39, 51, 72, 85	0
14	b	196/196 (100%)	-0.41	0 100 100	40, 51, 72, 85	0
All	All	6368/6368 (100%)	-0.25	98 (1%) 74 75	38, 58, 91, 133	0

The worst 5 of 98 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
7	U	6	ALA	11.1
4	D	123(E)	SER	11.0
4	D	123(D)	ALA	10.8
4	D	123(F)	GLY	9.3
10	X	193	GLN	9.1

## 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
15	1Y9	N	201	15/15	0.92	0.26	4.13	65,71,74,75	0
15	1Y9	Y	301	15/15	0.90	0.25	3.83	67,75,78,80	0
15	1Y9	b	201	15/15	0.92	0.26	2.72	65,73,76,80	0
15	1Y9	K	301	15/15	0.91	0.23	2.60	68,74,78,79	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.