



# wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 5, 2023 – 05:28 AM EDT

PDB ID : 3UN8  
Title : Yeast 20S proteasome in complex with PR-957 (epoxide)  
Authors : Huber, E.; Basler, M.; Schwab, R.; Heinemeyer, W.; Kirk, C.; Groettrup, M.; Groll, M.  
Deposited on : 2011-11-15  
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

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.35  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.35

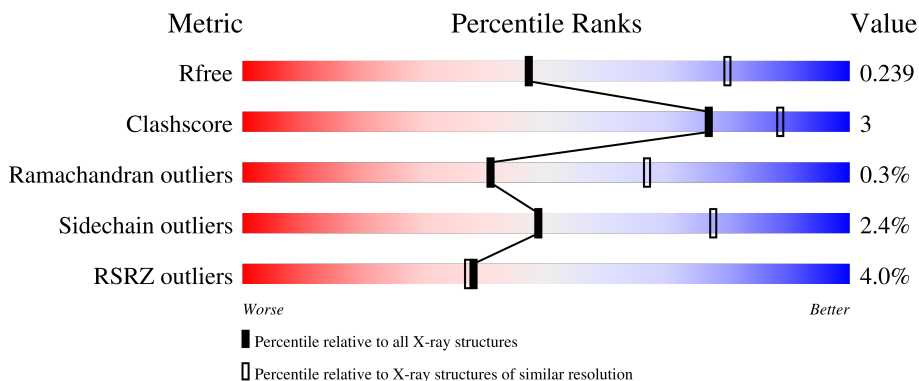
# 1 Overall quality at a glance

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))
$R_{free}$	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (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 of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	250	 4% 90% 10%
1	O	250	 4% 91% 9%
2	B	258	 6% 83% 11% • 5%
2	P	258	 7% 82% 11% • 5%
3	C	254	 9% 86% 8% • 5%

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Mol	Chain	Length	Quality of chain
3	Q	254	
4	D	260	
4	R	260	
5	E	234	
5	S	234	
6	F	288	
6	T	288	
7	G	252	
7	U	252	
8	H	232	
8	V	232	
9	I	205	
9	W	205	
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	

## 2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 50914 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
			Total	C	N	O	S			
1	A	250	1915	1219	315	377	4	0	0	0
1	O	250	1915	1219	315	377	4	0	0	0

- Molecule 2 is a protein called Proteasome component Y13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	244	1904	1201	321	379	3	0	0	0
2	P	244	1904	1201	321	379	3	0	0	0

- Molecule 3 is a protein called Proteasome component PRE6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	241	1890	1181	331	374	4	0	0	0
3	Q	241	1890	1181	331	374	4	0	0	0

- Molecule 4 is a protein called Proteasome component PUP2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	242	1861	1162	314	378	7	0	0	0
4	R	242	1861	1162	314	378	7	0	0	0

- 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
			1896	1205	330	357	4			
6	T	244	Total	C	N	O	S	0	0	0
			1896	1205	330	357	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			

- Molecule 8 is a protein called Proteasome component PUP1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	222	Total	C	N	O	S	0	0	0
			1684	1061	293	323	7			
8	V	222	Total	C	N	O	S	0	0	0
			1684	1061	293	323	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			

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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 component PRE2.

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.

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			

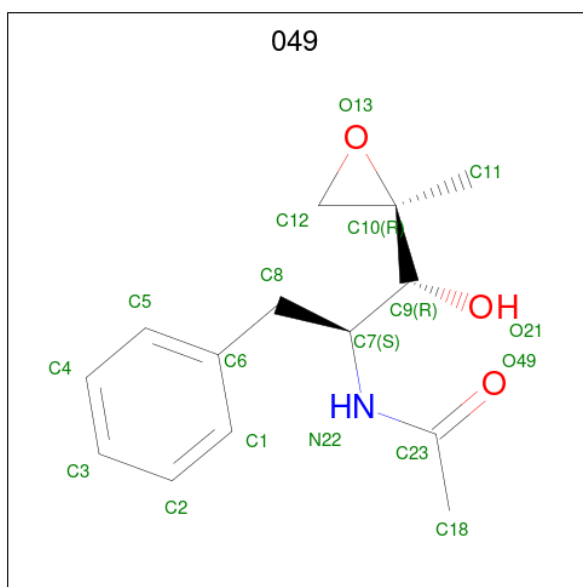
- Molecule 13 is a protein called Proteasome component PRE4.

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 component PRE3.

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 2-(acetylamino)-4,5-anhydro-1,2-dideoxy-4-methyl-1-phenyl-D-xylitol (three-letter code: 049) (formula: C<sub>14</sub>H<sub>19</sub>NO<sub>3</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
15	K	1	Total	C	N	O	0	0
			18	14	1	3		
15	Y	1	Total	C	N	O	0	0
			18	14	1	3		

- Molecule 16 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	A	61	Total	O	0	0
			61	61		
16	B	37	Total	O	0	0
			37	37		
16	C	42	Total	O	0	0
			42	42		
16	D	37	Total	O	0	0
			37	37		
16	E	21	Total	O	0	0
			21	21		
16	F	48	Total	O	0	0
			48	48		
16	G	60	Total	O	0	0
			60	60		
16	H	54	Total	O	0	0
			54	54		
16	I	65	Total	O	0	0
			65	65		
16	J	52	Total	O	0	0
			52	52		

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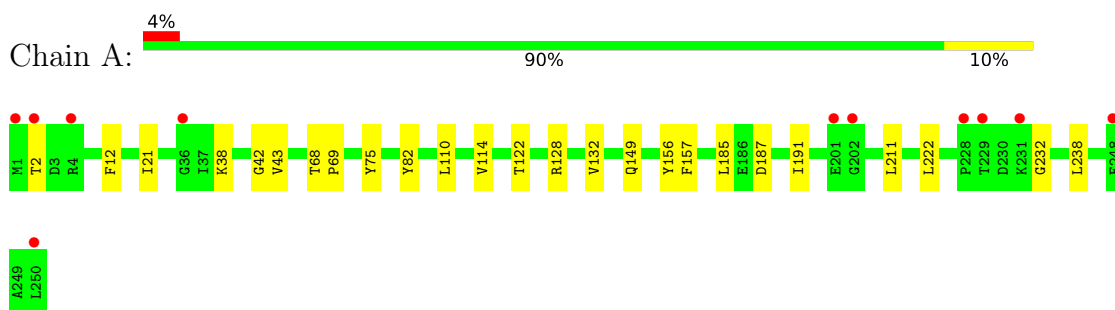
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	K	46	Total 46	O 46	0	0
16	L	56	Total 56	O 56	0	0
16	M	73	Total 73	O 73	0	0
16	N	58	Total 58	O 58	0	0
16	O	34	Total 34	O 34	0	0
16	P	29	Total 29	O 29	0	0
16	Q	28	Total 28	O 28	0	0
16	R	29	Total 29	O 29	0	0
16	S	20	Total 20	O 20	0	0
16	T	41	Total 41	O 41	0	0
16	U	61	Total 61	O 61	0	0
16	V	53	Total 53	O 53	0	0
16	W	60	Total 60	O 60	0	0
16	X	45	Total 45	O 45	0	0
16	Y	53	Total 53	O 53	0	0
16	Z	47	Total 47	O 47	0	0
16	a	73	Total 73	O 73	0	0
16	b	57	Total 57	O 57	0	0



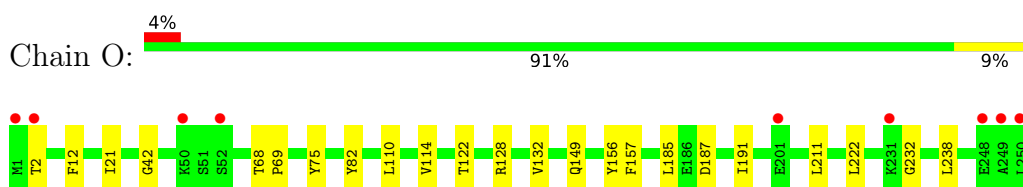
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

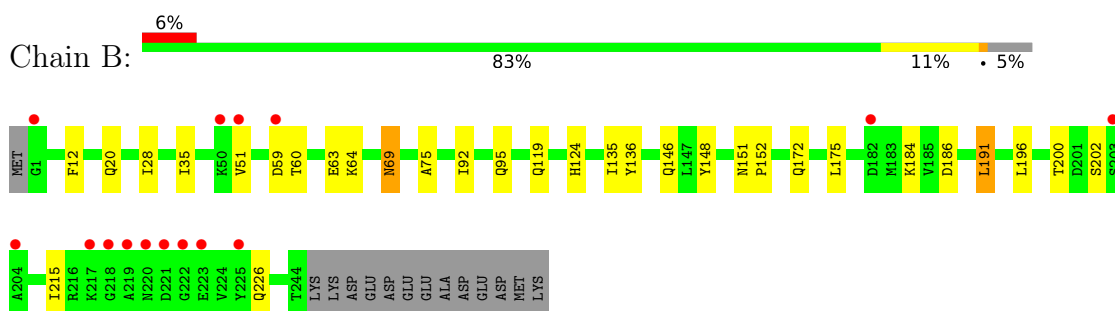
- Molecule 1: Proteasome component Y7



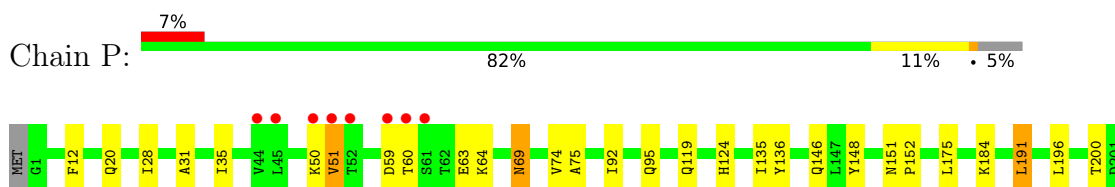
- Molecule 1: Proteasome component Y7

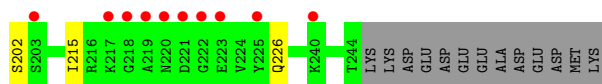


- Molecule 2: Proteasome component Y13

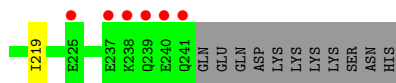
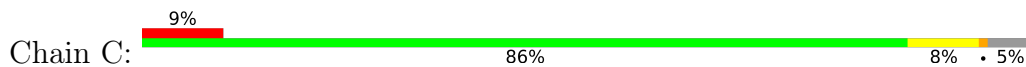


- Molecule 2: Proteasome component Y13

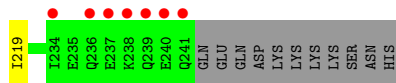
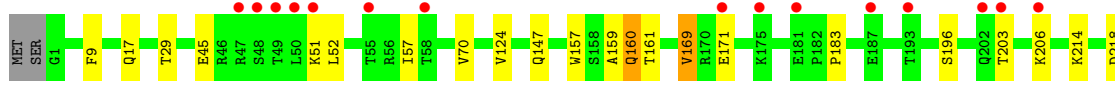
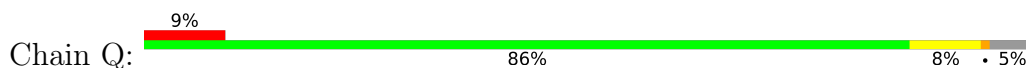




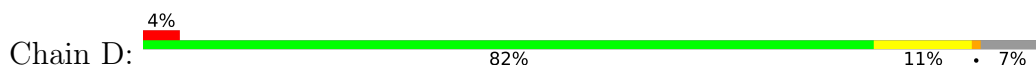
- Molecule 3: Proteasome component PRE6



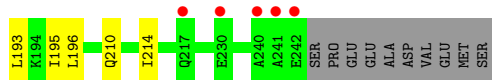
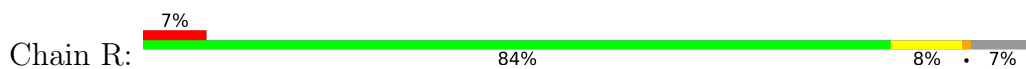
- Molecule 3: Proteasome component PRE6



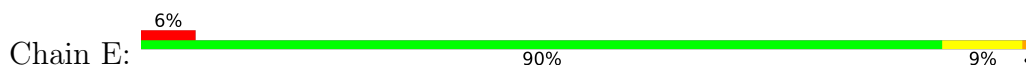
- Molecule 4: Proteasome component PUP2

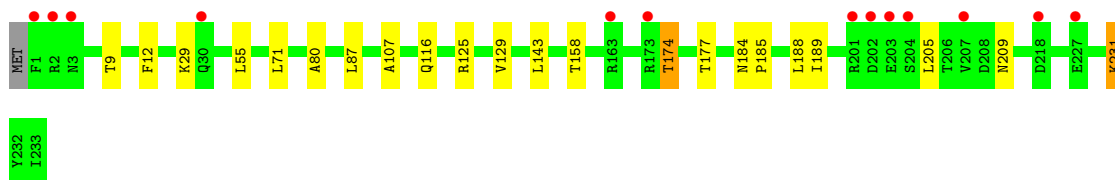


- Molecule 4: Proteasome component PUP2

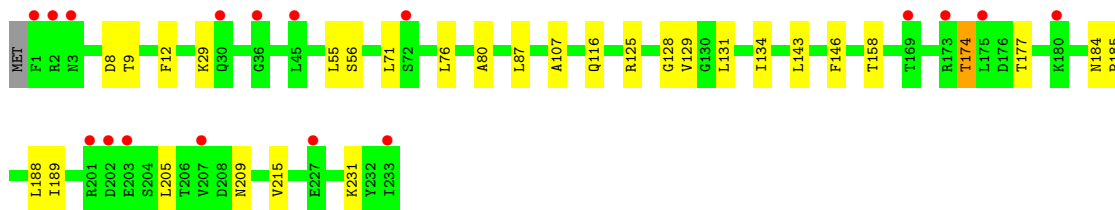
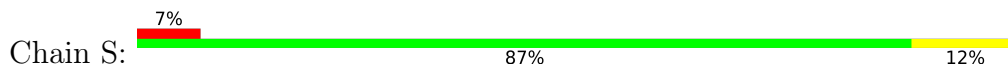


- Molecule 5: Proteasome component PRE5

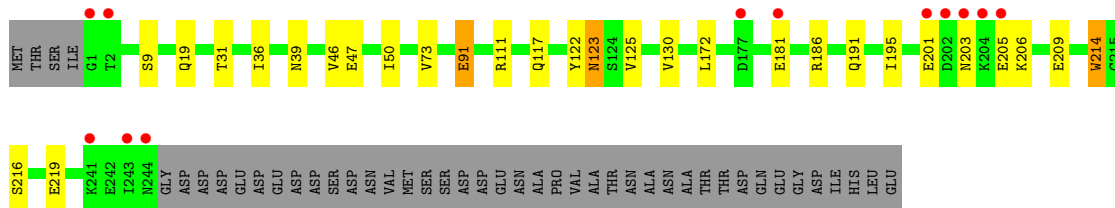
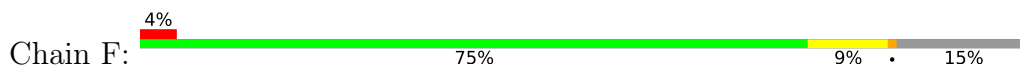




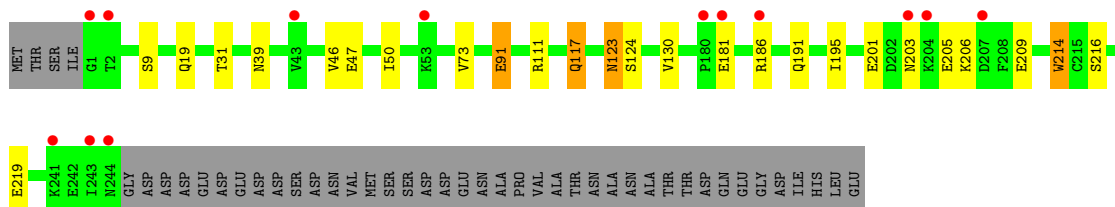
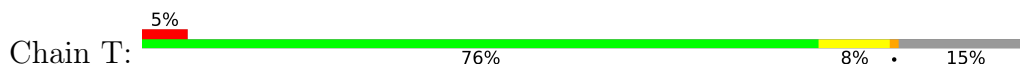
- Molecule 5: Proteasome component PRE5



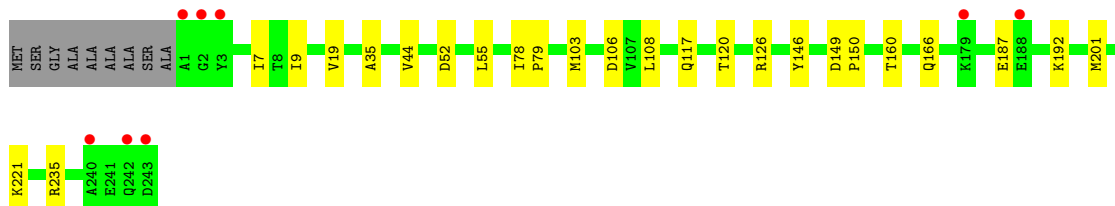
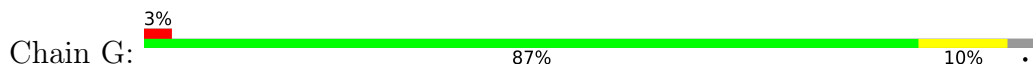
- Molecule 6: Proteasome component C1



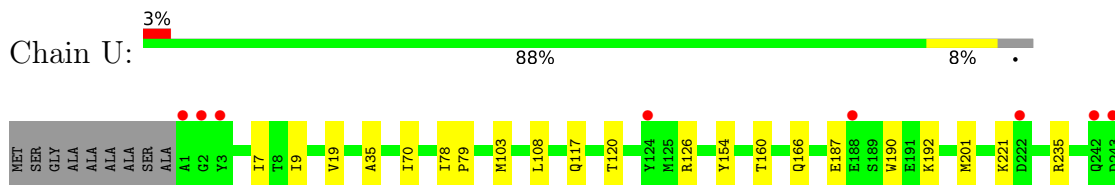
- Molecule 6: Proteasome component C1



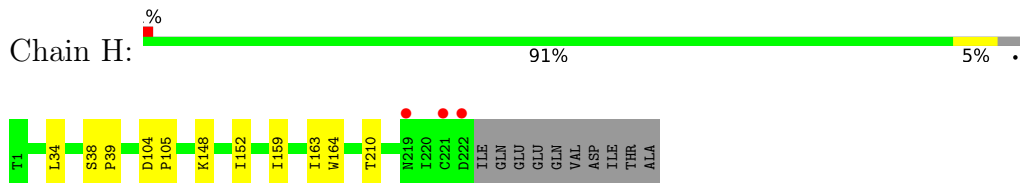
- Molecule 7: Proteasome component C7-alpha



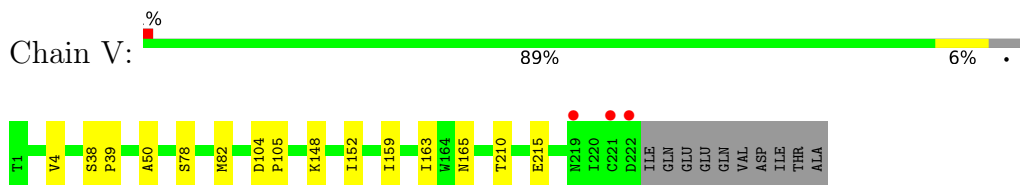
- Molecule 7: Proteasome component C7-alpha



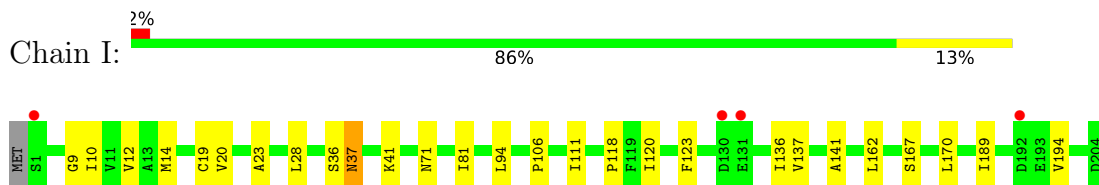
- Molecule 8: Proteasome component PUP1



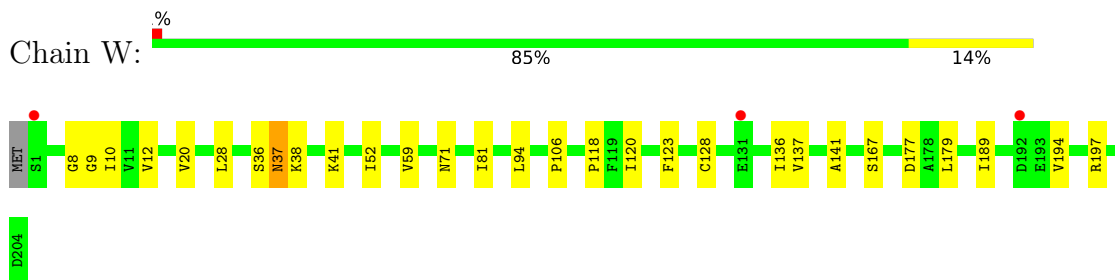
- Molecule 8: Proteasome component PUP1



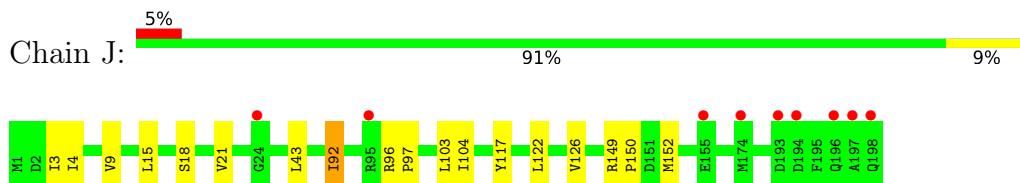
- Molecule 9: Proteasome component PUP3



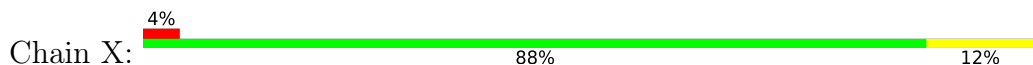
- Molecule 9: Proteasome component PUP3



- Molecule 10: Proteasome component C11

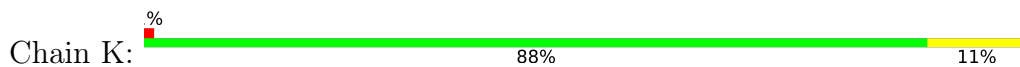


- Molecule 10: Proteasome component C11

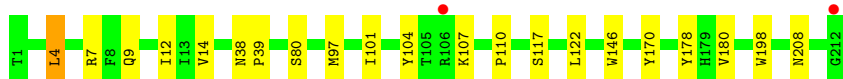
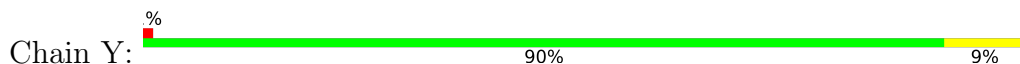




- Molecule 11: Proteasome component PRE2



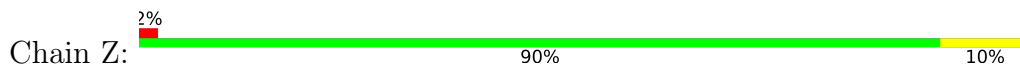
- Molecule 11: Proteasome component PRE2



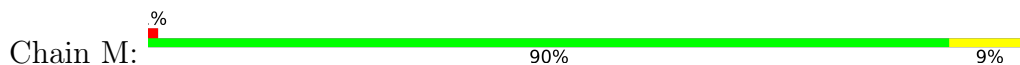
- Molecule 12: Proteasome component C5



- Molecule 12: Proteasome component C5



- Molecule 13: Proteasome component PRE4



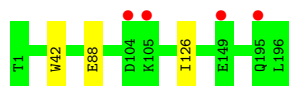
- Molecule 13: Proteasome component PRE4



- Molecule 14: Proteasome component PRE3



- Molecule 14: Proteasome component PRE3



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	135.42Å 300.42Å 143.93Å 90.00° 112.83° 90.00°	Depositor
Resolution (Å)	15.00 – 2.70 24.94 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.2 (15.00-2.70) 99.4 (24.94-2.70)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.93 (at 2.72Å)	Xtrriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.217 , 0.240 0.217 , 0.239	Depositor DCC
$R_{free}$ test set	14346 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	45.4	Xtrriage
Anisotropy	0.809	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 46.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	50914	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	54.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.18% 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:  
049

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	0.46	0/2642
1	O	0.36	0/1952	0.46	0/2642
2	B	0.33	0/1934	0.46	0/2618
2	P	0.33	0/1934	0.46	0/2618
3	C	0.34	0/1919	0.46	0/2598
3	Q	0.34	1/1919 (0.1%)	0.46	0/2598
4	D	0.36	0/1886	0.47	0/2541
4	R	0.36	1/1886 (0.1%)	0.47	0/2541
5	E	0.31	0/1823	0.45	0/2463
5	S	0.31	0/1823	0.44	0/2463
6	F	0.41	1/1936 (0.1%)	0.44	0/2614
6	T	0.41	1/1936 (0.1%)	0.44	0/2614
7	G	0.34	0/1959	0.46	0/2652
7	U	0.34	1/1959 (0.1%)	0.46	0/2652
8	H	0.44	1/1715 (0.1%)	0.46	0/2326
8	V	0.44	0/1715	0.46	0/2326
9	I	0.34	0/1611	0.47	0/2174
9	W	0.34	0/1611	0.47	0/2174
10	J	0.32	0/1613	0.45	0/2173
10	X	0.31	0/1613	0.45	0/2173
11	K	0.50	1/1681 (0.1%)	0.49	1/2274 (0.0%)
11	Y	0.51	2/1681 (0.1%)	0.50	1/2274 (0.0%)
12	L	0.36	0/1795	0.45	0/2420
12	Z	0.36	0/1795	0.45	0/2420
13	M	0.36	0/1855	0.47	0/2514
13	a	0.36	1/1855 (0.1%)	0.48	0/2514
14	N	0.39	0/1541	0.44	0/2087
14	b	0.39	1/1541 (0.1%)	0.45	0/2087
All	All	0.37	11/50440 (0.0%)	0.46	2/68192 (0.0%)

The worst 5 of 11 bond length outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	b	42	TRP	CD2-CE2	5.05	1.47	1.41
11	Y	146	TRP	CD2-CE2	5.04	1.47	1.41
4	R	179	TRP	CD2-CE2	5.04	1.47	1.41
6	F	214	TRP	CD2-CE2	5.03	1.47	1.41
3	Q	157	TRP	CD2-CE2	5.03	1.47	1.41

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
11	Y	4	LEU	CA-CB-CG	5.62	128.24	115.30
11	K	4	LEU	CA-CB-CG	5.59	128.15	115.30

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	1929	12	0
1	O	1915	0	1929	11	0
2	B	1904	0	1904	17	0
2	P	1904	0	1904	16	0
3	C	1890	0	1903	14	0
3	Q	1890	0	1903	11	0
4	D	1861	0	1839	13	0
4	R	1861	0	1839	12	0
5	E	1795	0	1800	10	0
5	S	1795	0	1800	14	0
6	F	1896	0	1889	14	0
6	T	1896	0	1889	13	0
7	G	1921	0	1913	11	0
7	U	1921	0	1913	9	0
8	H	1684	0	1688	6	0
8	V	1684	0	1688	10	0
9	I	1581	0	1574	17	0
9	W	1581	0	1574	19	0
10	J	1585	0	1590	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	X	1585	0	1590	14	0
11	K	1644	0	1594	16	0
11	Y	1644	0	1594	12	0
12	L	1757	0	1711	6	0
12	Z	1757	0	1711	11	0
13	M	1824	0	1832	12	0
13	a	1824	0	1832	0	0
14	N	1512	0	1481	2	0
14	b	1512	0	1481	0	0
15	K	18	0	17	3	0
15	Y	18	0	17	4	0
16	A	61	0	0	0	0
16	B	37	0	0	0	0
16	C	42	0	0	0	0
16	D	37	0	0	0	0
16	E	21	0	0	0	0
16	F	48	0	0	0	0
16	G	60	0	0	0	0
16	H	54	0	0	0	0
16	I	65	0	0	0	0
16	J	52	0	0	0	0
16	K	46	0	0	0	0
16	L	56	0	0	0	0
16	M	73	0	0	0	0
16	N	58	0	0	0	0
16	O	34	0	0	0	0
16	P	29	0	0	0	0
16	Q	28	0	0	0	0
16	R	29	0	0	0	0
16	S	20	0	0	0	0
16	T	41	0	0	0	0
16	U	61	0	0	0	0
16	V	53	0	0	0	0
16	W	60	0	0	0	0
16	X	45	0	0	0	0
16	Y	53	0	0	1	0
16	Z	47	0	0	0	0
16	a	73	0	0	0	0
16	b	57	0	0	0	0
All	All	50914	0	49328	275	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 3.

The worst 5 of 275 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:Y:170:TYR:HB3	15:Y:213:049:H12A	1.53	0.89
11:K:1:THR:CB	15:K:213:049:C9	2.51	0.87
12:L:109:THR:HG23	12:L:125:PHE:HB2	1.66	0.78
3:Q:160:GLN:HA	3:Q:160:GLN:HE21	1.50	0.76
3:C:160:GLN:HE21	3:C:160:GLN:HA	1.53	0.73

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%)	242 (98%)	5 (2%)	1 (0%)	34	60
1	O	248/250 (99%)	240 (97%)	7 (3%)	1 (0%)	34	60
2	B	242/258 (94%)	236 (98%)	5 (2%)	1 (0%)	34	60
2	P	242/258 (94%)	234 (97%)	7 (3%)	1 (0%)	34	60
3	C	239/254 (94%)	233 (98%)	3 (1%)	3 (1%)	12	30
3	Q	239/254 (94%)	232 (97%)	4 (2%)	3 (1%)	12	30
4	D	240/260 (92%)	235 (98%)	3 (1%)	2 (1%)	19	43
4	R	240/260 (92%)	234 (98%)	4 (2%)	2 (1%)	19	43
5	E	231/234 (99%)	227 (98%)	4 (2%)	0	100	100
5	S	231/234 (99%)	226 (98%)	5 (2%)	0	100	100
6	F	242/288 (84%)	235 (97%)	7 (3%)	0	100	100
6	T	242/288 (84%)	235 (97%)	7 (3%)	0	100	100
7	G	241/252 (96%)	233 (97%)	8 (3%)	0	100	100
7	U	241/252 (96%)	235 (98%)	6 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	H	220/232 (95%)	213 (97%)	7 (3%)	0	100	100
8	V	220/232 (95%)	214 (97%)	6 (3%)	0	100	100
9	I	202/205 (98%)	197 (98%)	5 (2%)	0	100	100
9	W	202/205 (98%)	194 (96%)	8 (4%)	0	100	100
10	J	196/198 (99%)	186 (95%)	9 (5%)	1 (0%)	29	54
10	X	196/198 (99%)	188 (96%)	7 (4%)	1 (0%)	29	54
11	K	210/212 (99%)	207 (99%)	3 (1%)	0	100	100
11	Y	210/212 (99%)	205 (98%)	5 (2%)	0	100	100
12	L	220/222 (99%)	214 (97%)	6 (3%)	0	100	100
12	Z	220/222 (99%)	215 (98%)	5 (2%)	0	100	100
13	M	231/233 (99%)	221 (96%)	9 (4%)	1 (0%)	34	60
13	a	231/233 (99%)	221 (96%)	9 (4%)	1 (0%)	34	60
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	6312/6588 (96%)	6130 (97%)	164 (3%)	18 (0%)	41	66

5 of 18 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	118	GLY
1	A	2	THR
3	C	52	LEU
3	C	203	THR
1	O	2	THR

### 5.3.2 Protein sidechains [i](#)

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%)	207 (99%)	2 (1%)	76	91
1	O	209/209 (100%)	207 (99%)	2 (1%)	76	91

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	203/216 (94%)	194 (96%)	9 (4%)	28	56
2	P	203/216 (94%)	194 (96%)	9 (4%)	28	56
3	C	213/226 (94%)	208 (98%)	5 (2%)	50	78
3	Q	213/226 (94%)	207 (97%)	6 (3%)	43	73
4	D	198/215 (92%)	190 (96%)	8 (4%)	31	60
4	R	198/215 (92%)	193 (98%)	5 (2%)	47	76
5	E	192/193 (100%)	184 (96%)	8 (4%)	30	58
5	S	192/193 (100%)	183 (95%)	9 (5%)	26	54
6	F	201/239 (84%)	191 (95%)	10 (5%)	24	51
6	T	201/239 (84%)	191 (95%)	10 (5%)	24	51
7	G	207/210 (99%)	201 (97%)	6 (3%)	42	71
7	U	207/210 (99%)	201 (97%)	6 (3%)	42	71
8	H	181/190 (95%)	180 (99%)	1 (1%)	86	95
8	V	181/190 (95%)	180 (99%)	1 (1%)	86	95
9	I	172/173 (99%)	170 (99%)	2 (1%)	71	88
9	W	172/173 (99%)	170 (99%)	2 (1%)	71	88
10	J	175/175 (100%)	174 (99%)	1 (1%)	86	95
10	X	175/175 (100%)	174 (99%)	1 (1%)	86	95
11	K	169/169 (100%)	165 (98%)	4 (2%)	49	77
11	Y	169/169 (100%)	166 (98%)	3 (2%)	59	83
12	L	185/185 (100%)	183 (99%)	2 (1%)	73	90
12	Z	185/185 (100%)	183 (99%)	2 (1%)	73	90
13	M	199/199 (100%)	192 (96%)	7 (4%)	36	65
13	a	199/199 (100%)	193 (97%)	6 (3%)	41	70
14	N	162/162 (100%)	161 (99%)	1 (1%)	86	95
14	b	162/162 (100%)	160 (99%)	2 (1%)	71	88
All	All	5332/5522 (97%)	5202 (98%)	130 (2%)	49	77

5 of 130 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
9	W	81	ILE
11	Y	104	TYR

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Mol	Chain	Res	Type
8	H	34	LEU
7	G	235	ARG
12	Z	128	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 126 such sidechains are listed below:

Mol	Chain	Res	Type
13	M	108	ASN
11	Y	85	ASN
3	Q	17	GLN
11	Y	62	GLN
12	Z	195	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 monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

2 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	049	Y	213	11	18,19,19	3.00	6 (33%)	23,27,27	4.33	9 (39%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
15	049	K	213	11	18,19,19	3.23	6 (33%)	23,27,27	4.17	10 (43%)

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	049	Y	213	11	-	9/18/22/22	0/2/2/2
15	049	K	213	11	-	5/18/22/22	0/2/2/2

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	Y	213	049	C8-C7	-8.90	1.35	1.53
15	K	213	049	C8-C7	-8.86	1.35	1.53
15	K	213	049	C9-C7	-6.29	1.46	1.53
15	K	213	049	C12-C10	5.15	1.59	1.46
15	Y	213	049	C12-C10	5.14	1.59	1.46

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	Y	213	049	C8-C7-C9	12.61	132.80	111.70
15	K	213	049	C8-C7-C9	12.02	131.81	111.70
15	Y	213	049	C10-C9-C7	-10.02	92.36	115.71
15	Y	213	049	C12-O13-C10	8.88	69.31	60.44
15	K	213	049	C12-O13-C10	8.72	69.15	60.44

There are no chirality outliers.

5 of 14 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	K	213	049	C8-C7-C9-C10
15	K	213	049	C8-C7-C9-O21
15	Y	213	049	C8-C7-C9-O21
15	Y	213	049	N22-C7-C9-C10
15	Y	213	049	N22-C7-C9-O21

There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	Y	213	049	4	0
15	K	213	049	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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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%)	0.05	11 (4%) 34 33	34, 48, 77, 99	0
1	O	250/250 (100%)	0.15	9 (3%) 42 42	38, 54, 87, 111	0
2	B	244/258 (94%)	0.22	15 (6%) 21 20	34, 52, 81, 112	0
2	P	244/258 (94%)	0.35	18 (7%) 14 12	38, 54, 87, 116	0
3	C	241/254 (94%)	0.36	23 (9%) 8 6	36, 56, 105, 147	0
3	Q	241/254 (94%)	0.40	22 (9%) 9 7	40, 63, 119, 160	0
4	D	242/260 (93%)	0.27	10 (4%) 37 36	41, 55, 83, 110	0
4	R	242/260 (93%)	0.39	19 (7%) 12 10	42, 60, 94, 115	0
5	E	233/234 (99%)	0.19	13 (5%) 24 23	41, 58, 86, 101	0
5	S	233/234 (99%)	0.36	17 (7%) 15 13	45, 62, 91, 104	0
6	F	244/288 (84%)	0.15	12 (4%) 29 28	38, 55, 89, 113	0
6	T	244/288 (84%)	0.23	13 (5%) 26 25	37, 57, 92, 119	0
7	G	243/252 (96%)	-0.07	8 (3%) 46 46	35, 50, 79, 120	0
7	U	243/252 (96%)	0.03	8 (3%) 46 46	38, 50, 75, 115	0
8	H	222/232 (95%)	0.02	3 (1%) 75 77	38, 48, 68, 100	0
8	V	222/232 (95%)	-0.03	3 (1%) 75 77	37, 49, 68, 101	0
9	I	204/205 (99%)	-0.17	4 (1%) 65 67	34, 45, 66, 75	0
9	W	204/205 (99%)	-0.11	3 (1%) 73 76	36, 47, 68, 83	0
10	J	198/198 (100%)	-0.03	9 (4%) 33 31	35, 47, 66, 116	0
10	X	198/198 (100%)	-0.01	7 (3%) 44 44	39, 49, 65, 111	0
11	K	212/212 (100%)	-0.13	2 (0%) 84 85	33, 43, 63, 70	0
11	Y	212/212 (100%)	-0.07	2 (0%) 84 85	35, 46, 66, 75	0
12	L	222/222 (100%)	-0.15	5 (2%) 60 62	34, 46, 73, 85	0
12	Z	222/222 (100%)	-0.09	4 (1%) 68 70	35, 47, 72, 87	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	M	233/233 (100%)	-0.17	3 (1%) 77 78	33, 47, 69, 85	0
13	a	233/233 (100%)	-0.18	2 (0%) 84 85	32, 46, 64, 77	0
14	N	196/196 (100%)	-0.21	3 (1%) 73 76	33, 43, 64, 79	0
14	b	196/196 (100%)	-0.18	4 (2%) 65 67	34, 45, 64, 75	0
All	All	6368/6588 (96%)	0.07	252 (3%) 38 37	32, 50, 85, 160	0

The worst 5 of 252 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	R	121	GLY	11.7
4	R	119	ALA	10.2
3	C	50	LEU	9.4
3	C	49	THR	9.4
4	D	119	ALA	9.3

## 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 monosaccharides 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	049	K	213	18/18	0.82	0.29	35,40,41,42	0
15	049	Y	213	18/18	0.84	0.25	38,42,43,44	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.