



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 20, 2026 – 12:08 AM UTC

PDB ID : 1IRU / pdb_00001iru
Title : Crystal Structure of the mammalian 20S proteasome at 2.75 Å resolution
Authors : Unno, M.; Mizushima, T.; Morimoto, Y.; Tomisugi, Y.; Tanaka, K.; Yasuoka, N.; Tsukihara, T.
Deposited on : 2001-10-24
Resolution : 2.75 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

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>.

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

MolProbity : 4-5-2 with Phenix2.0
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

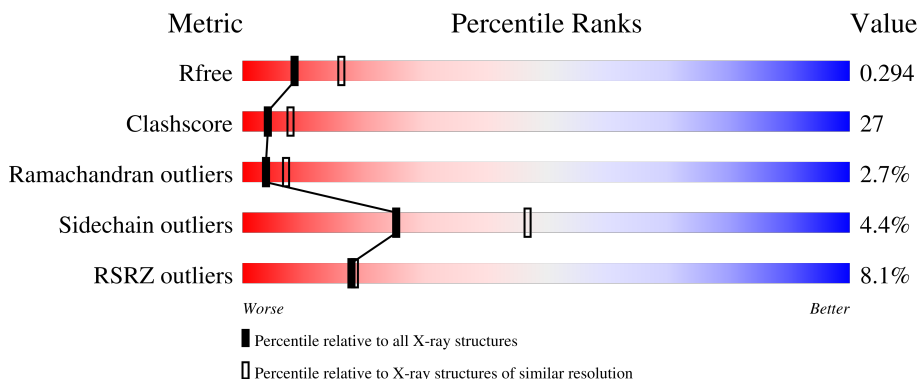
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 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}	180053	1009 (2.76-2.76)
Clashscore	190562	1044 (2.76-2.76)
Ramachandran outliers	187476	1024 (2.76-2.76)
Sidechain outliers	187428	1024 (2.76-2.76)
RSRZ outliers	180081	1009 (2.76-2.76)

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 ≥ 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	246	
1	O	246	
2	B	233	
2	P	233	
3	C	261	

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Mol	Chain	Length	Quality of chain
3	Q	261	
4	D	248	
4	R	248	
5	E	241	
5	S	241	
6	F	263	
6	T	263	
7	G	254	
7	U	254	
8	H	205	
8	V	205	
9	I	234	
9	W	234	
10	J	205	
10	X	205	
11	K	201	
11	Y	201	
12	L	204	
12	Z	204	
13	1	213	
13	M	213	
14	2	219	
14	N	219	

2 Entry composition [i](#)

There are 16 unique types of molecules in this entry. The entry contains 47757 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 20S proteasome.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	244	1842	1170	309	350	13	0	0	0
1	O	244	1842	1170	309	350	13	0	0	0

- Molecule 2 is a protein called 20S proteasome.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	233	1707	1081	287	334	5	0	0	0
2	P	233	1707	1081	287	334	5	0	0	0

- Molecule 3 is a protein called 20S proteasome.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	250	1902	1195	329	370	8	0	0	0
3	Q	250	1902	1195	329	370	8	0	0	0

- Molecule 4 is a protein called 20S proteasome.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	243	1665	1032	307	322	4	0	0	0
4	R	243	1665	1032	307	322	4	0	0	0

- Molecule 5 is a protein called 20S proteasome.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	234	Total	C	N	O	S	0	0	0
			1763	1104	290	358	11			
5	S	234	Total	C	N	O	S	0	0	0
			1763	1104	290	358	11			

- Molecule 6 is a protein called 20S proteasome.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	238	Total	C	N	O	S	0	0	0
			1850	1159	334	346	11			
6	T	238	Total	C	N	O	S	0	0	0
			1850	1159	334	346	11			

- Molecule 7 is a protein called 20S proteasome.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	245	Total	C	N	O	S	0	0	0
			1885	1195	319	360	11			
7	U	245	Total	C	N	O	S	0	0	0
			1885	1195	319	360	11			

- Molecule 8 is a protein called 20S proteasome.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	202	Total	C	N	O	S	0	0	0
			1509	945	258	294	12			
8	V	202	Total	C	N	O	S	0	0	0
			1509	945	258	294	12			

- Molecule 9 is a protein called 20S proteasome.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	220	Total	C	N	O	S	0	0	0
			1645	1034	282	317	12			
9	W	220	Total	C	N	O	S	0	0	0
			1645	1034	282	317	12			

- Molecule 10 is a protein called 20S proteasome.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	204	Total	C	N	O	S	0	0	0
			1585	1011	262	294	18			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	X	204	Total	C	N	O	S	0	0	0
			1585	1011	262	294	18			

- Molecule 11 is a protein called 20S proteasome.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	199	Total	C	N	O	S	0	0	0
			1570	1006	265	290	9			
11	Y	199	Total	C	N	O	S	0	0	0
			1570	1006	265	290	9			

- Molecule 12 is a protein called 20S proteasome.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	201	Total	C	N	O	S	0	0	0
			1548	974	273	292	9			
12	Z	201	Total	C	N	O	S	0	0	0
			1548	974	273	292	9			

- Molecule 13 is a protein called 20S proteasome.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	213	Total	C	N	O	S	0	0	0
			1639	1034	282	313	10			
13	1	213	Total	C	N	O	S	0	0	0
			1639	1034	282	313	10			

- Molecule 14 is a protein called 20S proteasome.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	N	217	Total	C	N	O	S	0	0	0
			1671	1053	287	319	12			
14	2	217	Total	C	N	O	S	0	0	0
			1671	1053	287	319	12			

- Molecule 15 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	A	1	Total	Mg	0	0
			1	1		
15	B	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	C	1	Total Mg 1 1	0	0
15	D	1	Total Mg 1 1	0	0
15	G	3	Total Mg 3 3	0	0
15	I	1	Total Mg 1 1	0	0
15	J	4	Total Mg 4 4	0	0
15	K	1	Total Mg 1 1	0	0
15	M	2	Total Mg 2 2	0	0
15	O	1	Total Mg 1 1	0	0
15	P	1	Total Mg 1 1	0	0
15	Q	1	Total Mg 1 1	0	0
15	R	1	Total Mg 1 1	0	0
15	U	3	Total Mg 3 3	0	0
15	W	1	Total Mg 1 1	0	0
15	X	4	Total Mg 4 4	0	0
15	Y	1	Total Mg 1 1	0	0
15	1	2	Total Mg 2 2	0	0

- Molecule 16 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	A	2	Total O 2 2	0	0
16	B	3	Total O 3 3	0	0
16	C	3	Total O 3 3	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	F	6	Total O 6 6	0	0
16	G	4	Total O 4 4	0	0
16	H	7	Total O 7 7	0	0
16	I	6	Total O 6 6	0	0
16	J	1	Total O 1 1	0	0
16	K	6	Total O 6 6	0	0
16	L	8	Total O 8 8	0	0
16	M	10	Total O 10 10	0	0
16	N	9	Total O 9 9	0	0
16	O	7	Total O 7 7	0	0
16	P	6	Total O 6 6	0	0
16	Q	3	Total O 3 3	0	0
16	R	3	Total O 3 3	0	0
16	S	1	Total O 1 1	0	0
16	T	7	Total O 7 7	0	0
16	U	9	Total O 9 9	0	0
16	V	15	Total O 15 15	0	0
16	W	9	Total O 9 9	0	0
16	X	17	Total O 17 17	0	0
16	Y	3	Total O 3 3	0	0
16	Z	8	Total O 8 8	0	0

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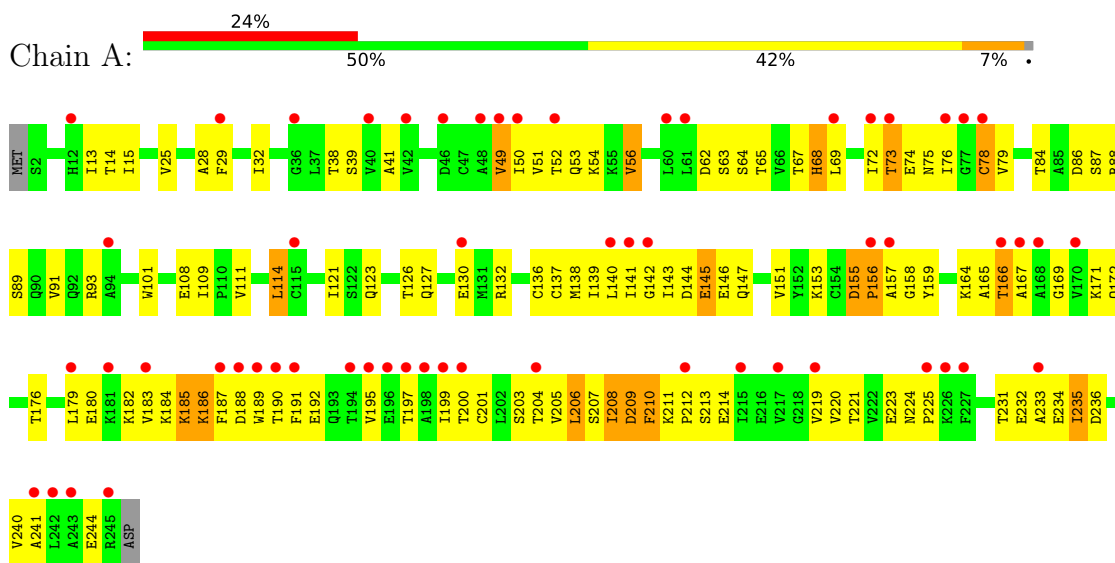
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	1	4	Total O 4 4	0	0
16	2	8	Total O 8 8	0	0

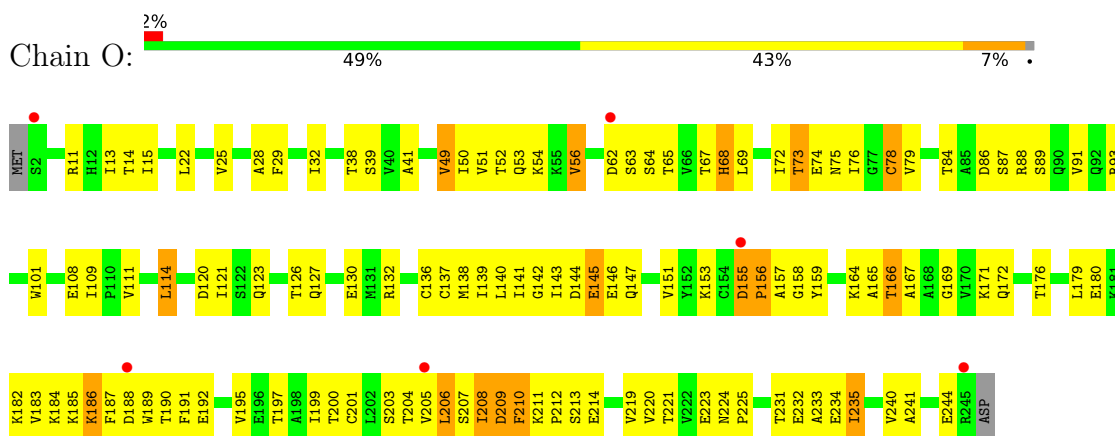
3 Residue-property plots [i](#)

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: 20S proteasome

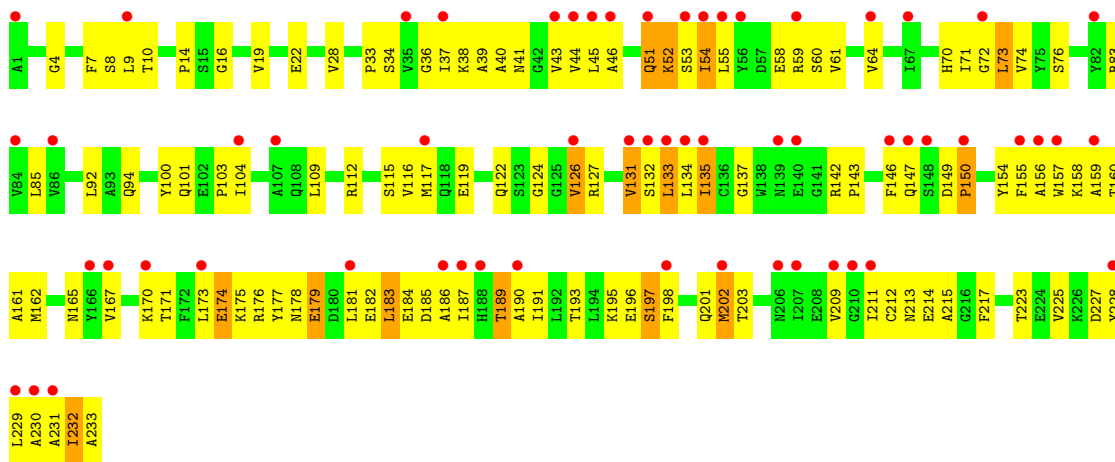


- Molecule 1: 20S proteasome

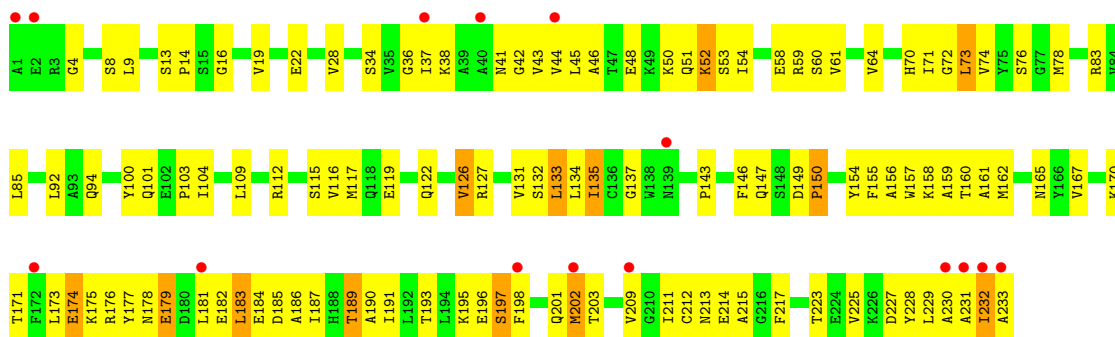


- Molecule 2: 20S proteasome

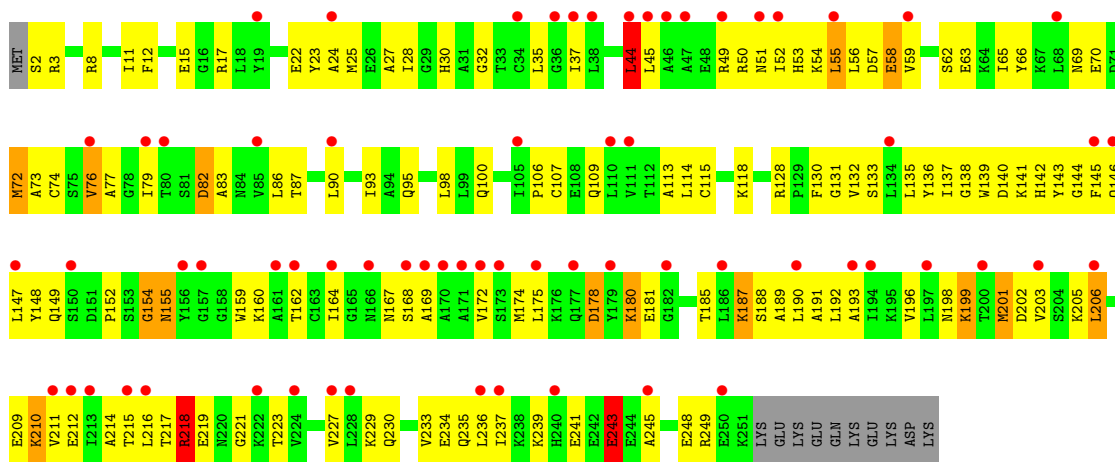




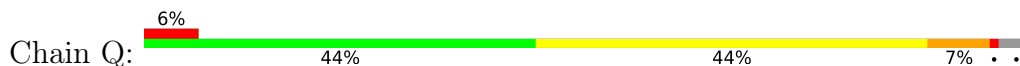
- Molecule 2: 20S proteasome

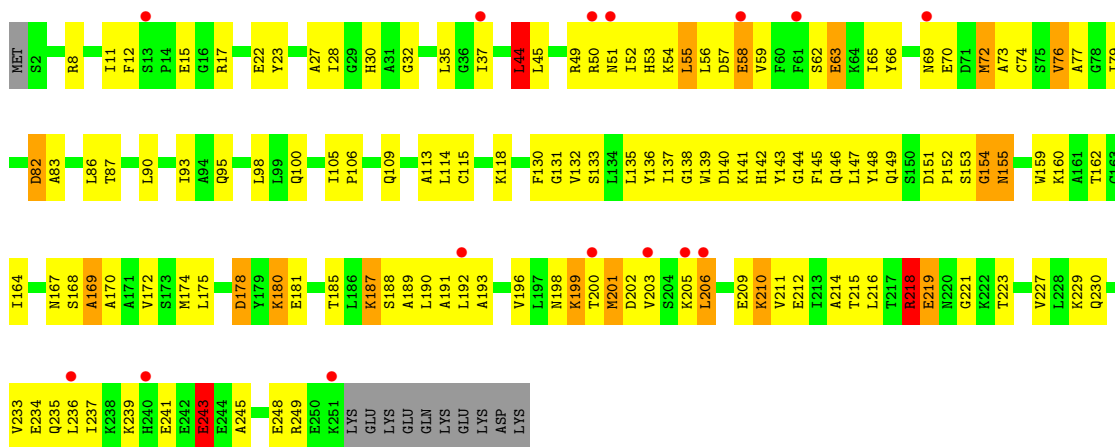


- Molecule 3: 20S proteasome

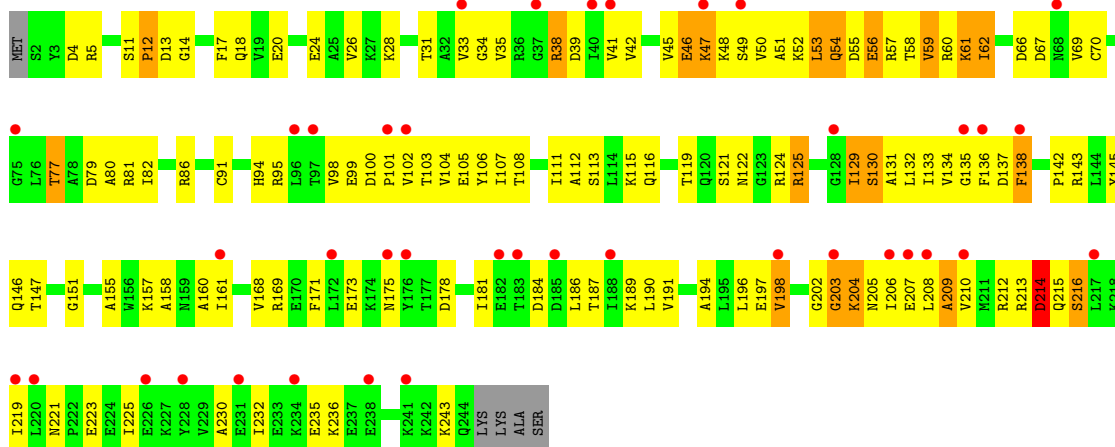


- Molecule 3: 20S proteasome

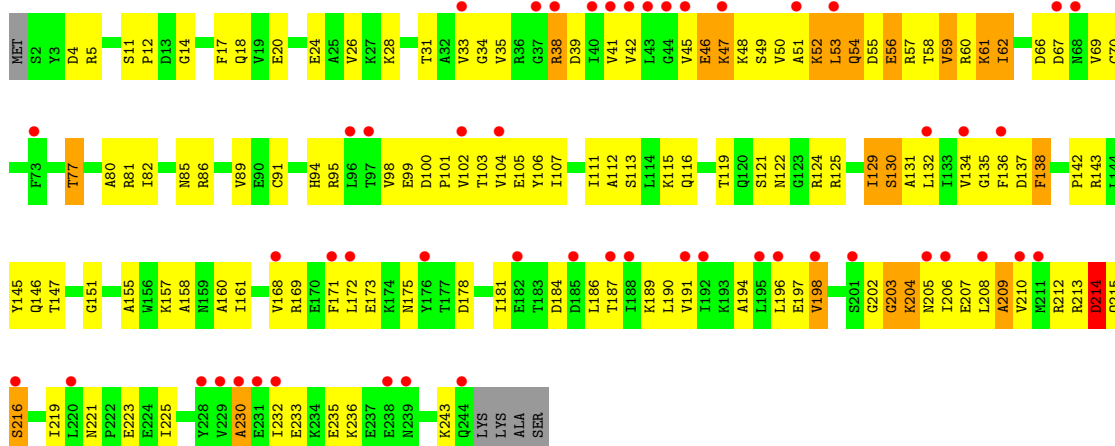
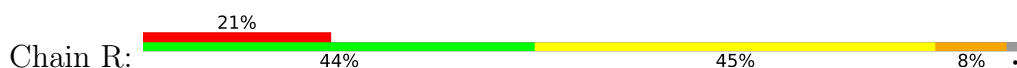




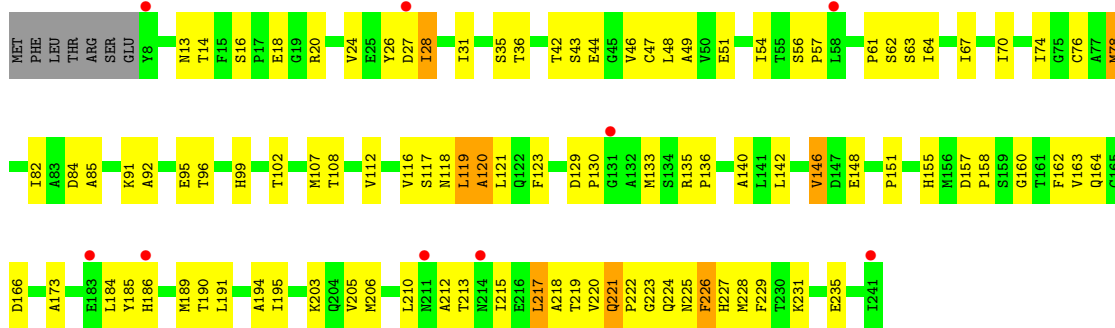
• Molecule 4: 20S proteasome



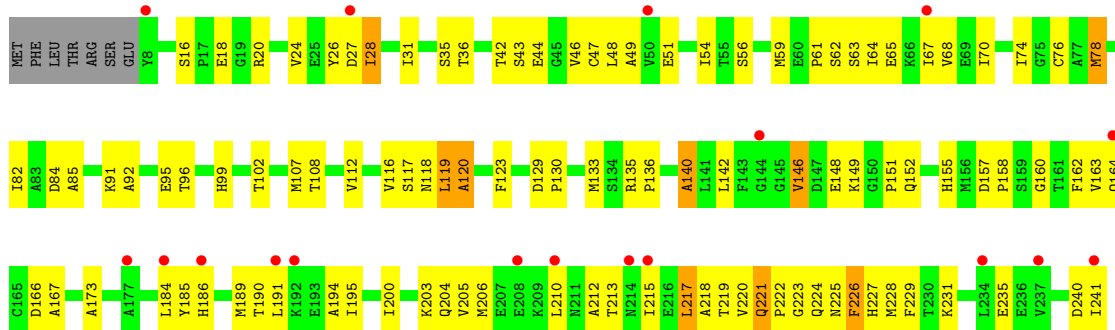
• Molecule 4: 20S proteasome



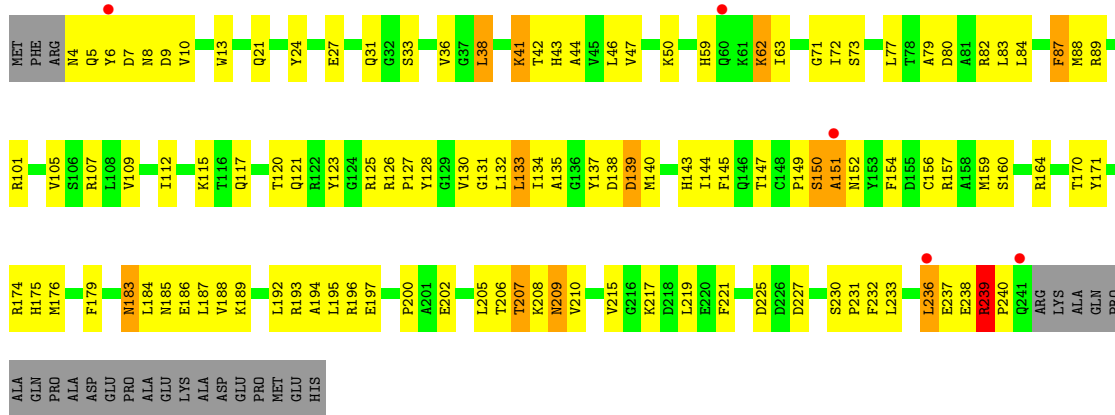
• Molecule 5: 20S proteasome



• Molecule 5: 20S proteasome

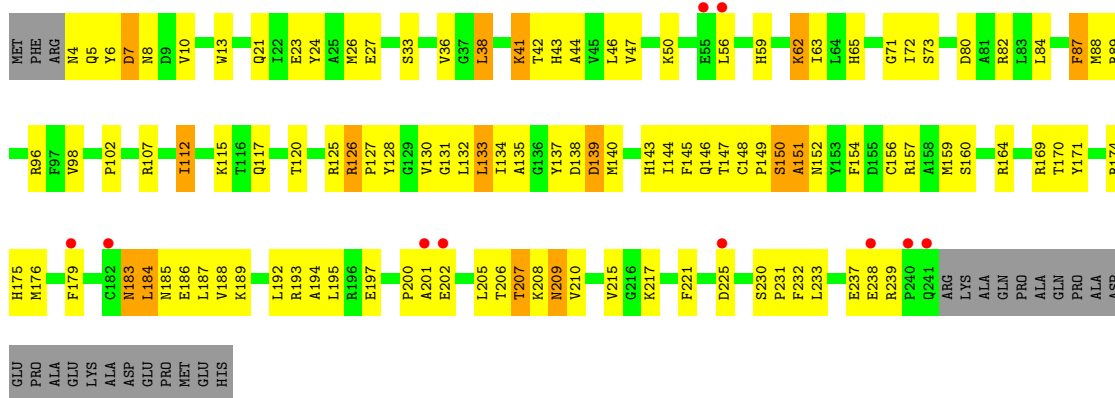


• Molecule 6: 20S proteasome

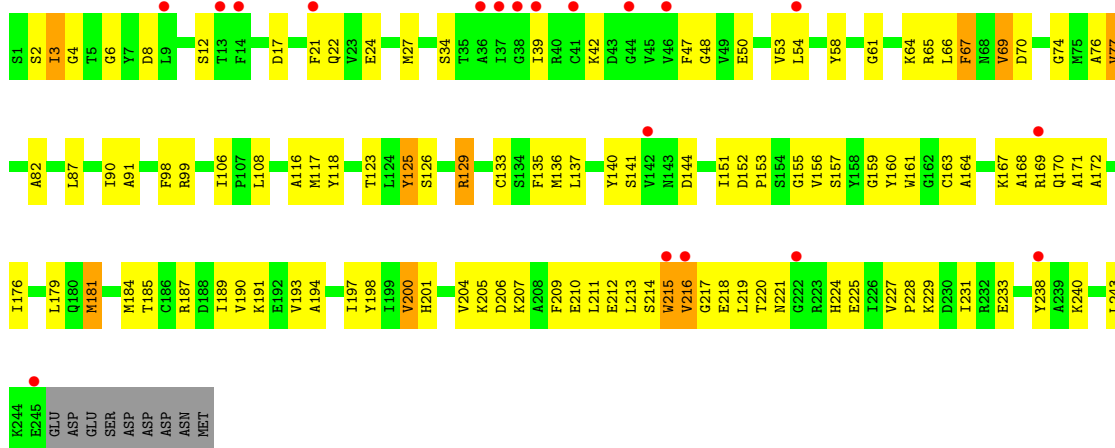


• Molecule 6: 20S proteasome

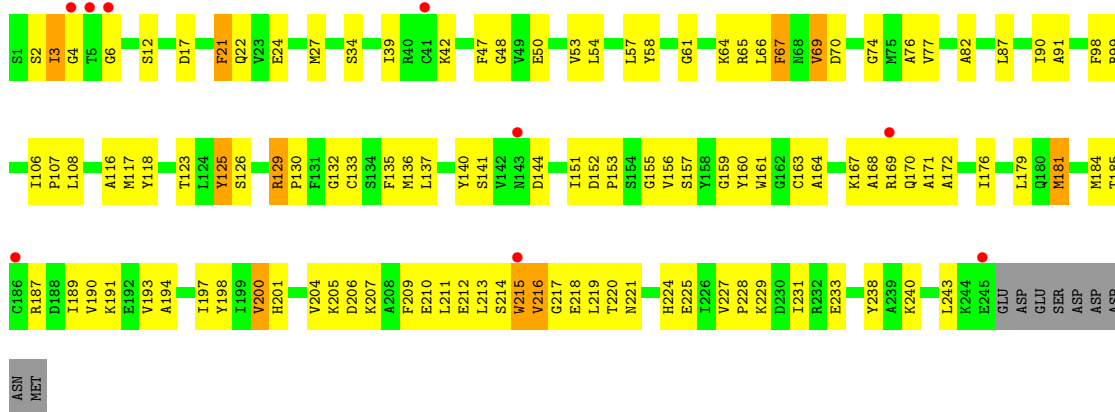




• Molecule 7: 20S proteasome



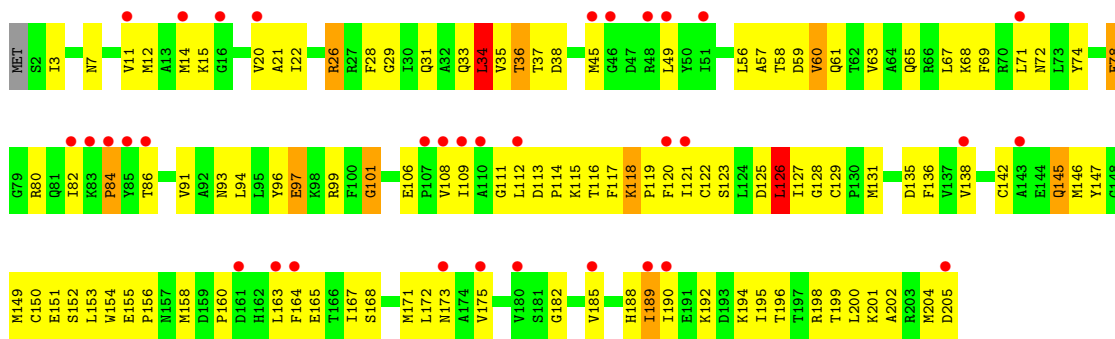
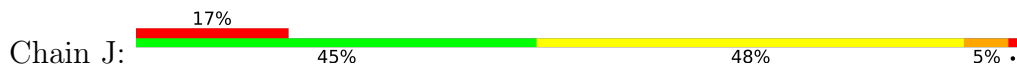
• Molecule 7: 20S proteasome



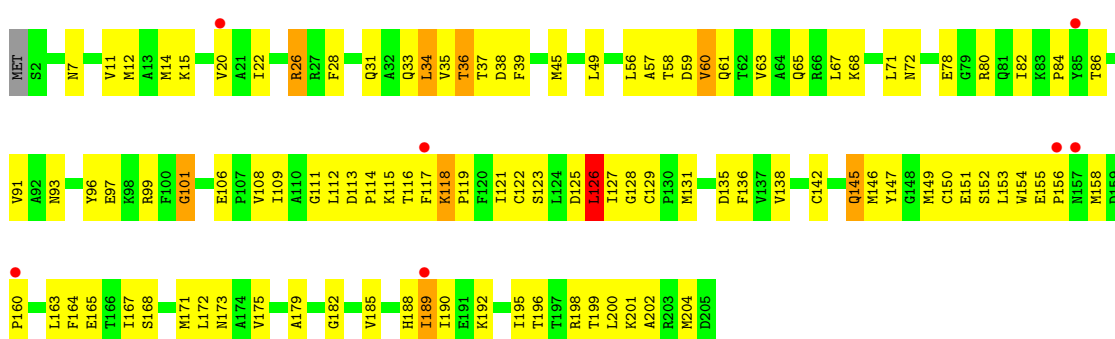
• Molecule 8: 20S proteasome



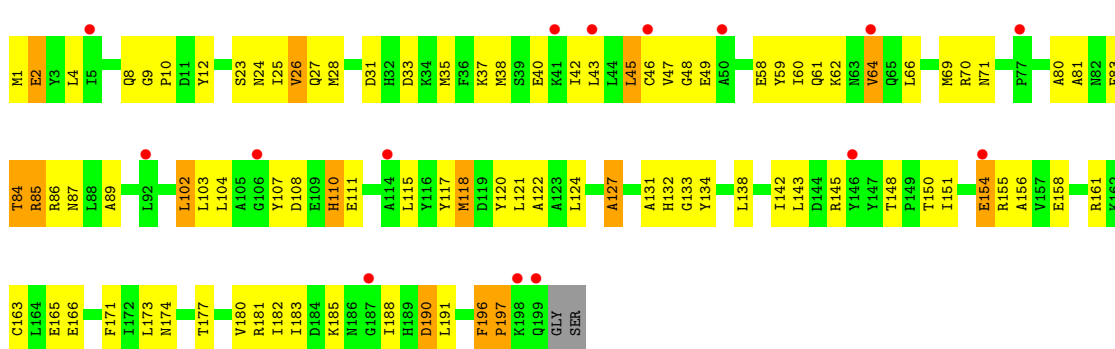
• Molecule 10: 20S proteasome



• Molecule 10: 20S proteasome

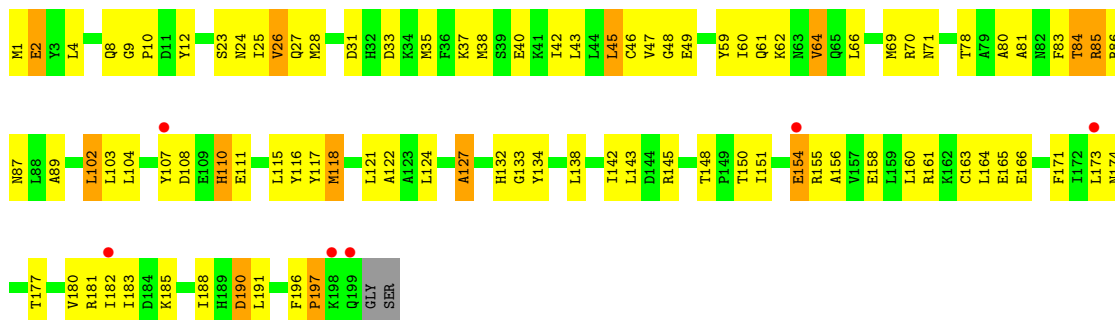


• Molecule 11: 20S proteasome

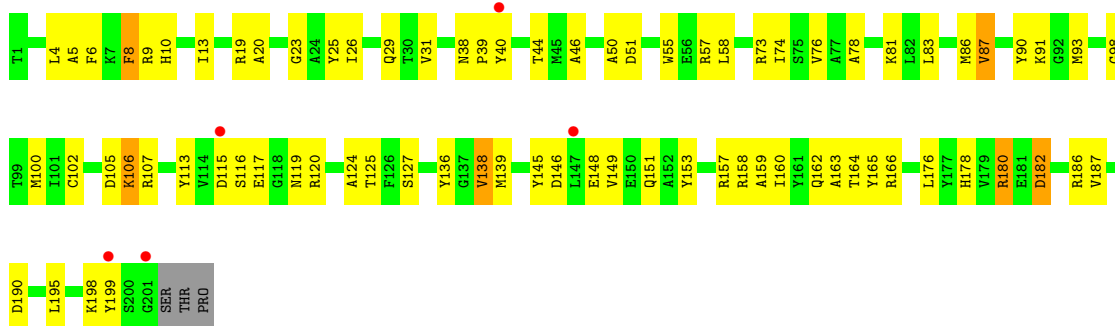


• Molecule 11: 20S proteasome

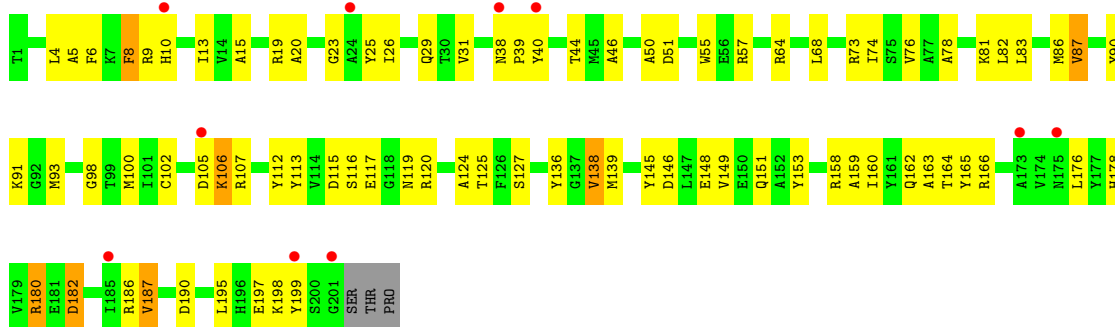




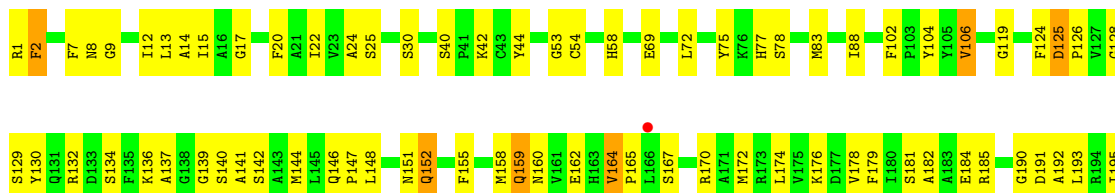
- Molecule 12: 20S proteasome



- Molecule 12: 20S proteasome

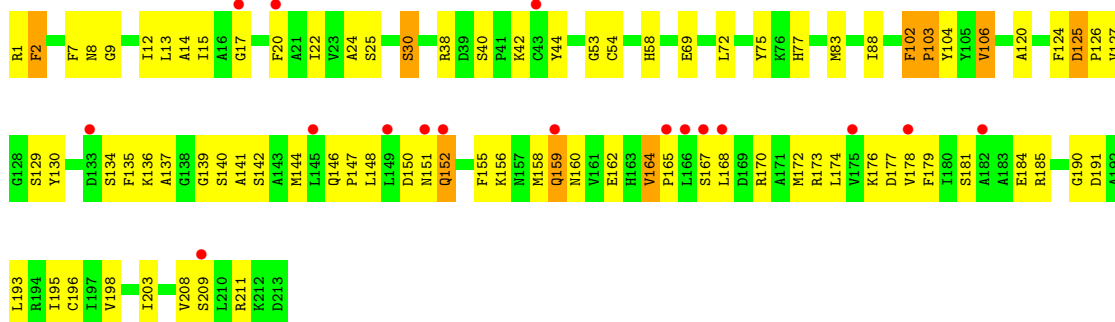


- Molecule 13: 20S proteasome

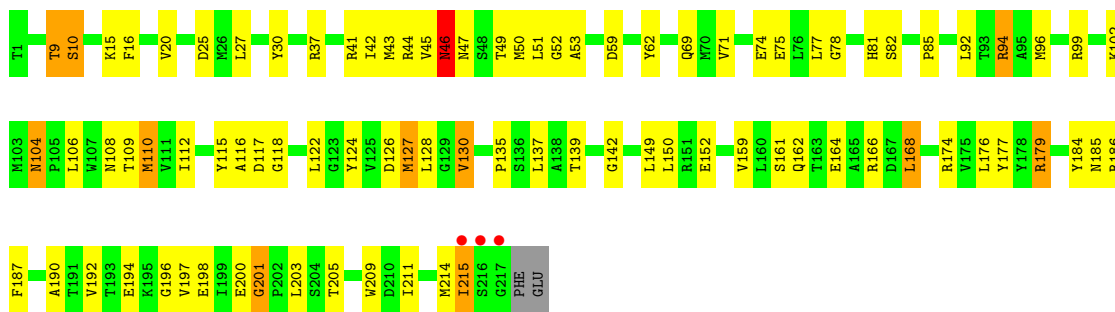




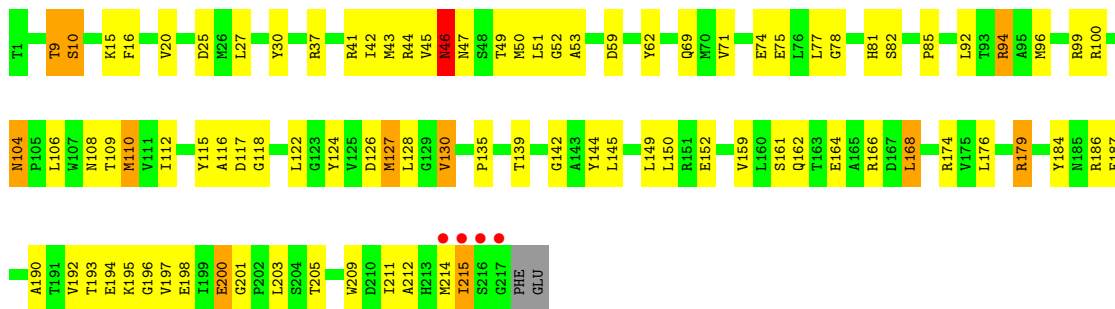
• Molecule 13: 20S proteasome



• Molecule 14: 20S proteasome



• Molecule 14: 20S proteasome



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	316.70Å 205.90Å 116.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	65.00 – 2.75 65.00 – 2.75	Depositor EDS
% Data completeness (in resolution range)	(Not available) (65.00-2.75) 96.1 (65.00-2.75)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.09 (at 2.73Å)	Xtrriage
Refinement program	CNS	Depositor
R, R_{free}	0.250 , 0.294 0.249 , 0.294	Depositor DCC
R_{free} test set	9420 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	67.6	Xtrriage
Anisotropy	0.397	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 51.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	47757	wwPDB-VP
Average B, all atoms (Å ²)	69.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.96% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: MG

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	0.43	0/1875	1.03	13/2545 (0.5%)
1	O	0.51	0/1875	1.03	12/2545 (0.5%)
2	B	0.40	0/1742	0.95	4/2372 (0.2%)
2	P	0.47	0/1742	0.97	5/2372 (0.2%)
3	C	0.38	0/1931	0.98	10/2613 (0.4%)
3	Q	0.44	0/1931	0.99	11/2613 (0.4%)
4	D	0.42	0/1688	1.00	10/2310 (0.4%)
4	R	0.46	0/1688	1.02	13/2310 (0.6%)
5	E	0.51	0/1790	0.99	8/2424 (0.3%)
5	S	0.49	0/1790	0.98	9/2424 (0.4%)
6	F	0.49	0/1885	1.07	16/2552 (0.6%)
6	T	0.49	0/1885	1.06	14/2552 (0.5%)
7	G	0.47	0/1920	0.99	7/2591 (0.3%)
7	U	0.54	0/1920	1.01	8/2591 (0.3%)
8	H	0.54	0/1535	0.97	1/2078 (0.0%)
8	V	0.56	0/1535	0.97	1/2078 (0.0%)
9	I	0.49	0/1672	1.06	10/2267 (0.4%)
9	W	0.53	0/1672	1.07	10/2267 (0.4%)
10	J	0.48	0/1614	1.08	16/2178 (0.7%)
10	X	0.56	0/1614	1.11	13/2178 (0.6%)
11	K	0.50	0/1603	1.05	14/2174 (0.6%)
11	Y	0.53	0/1603	1.06	13/2174 (0.6%)
12	L	0.54	0/1579	1.00	5/2134 (0.2%)
12	Z	0.52	0/1579	1.00	5/2134 (0.2%)
13	1	0.49	0/1669	0.99	9/2250 (0.4%)
13	M	0.55	0/1669	1.00	9/2250 (0.4%)
14	2	0.53	0/1704	1.05	12/2311 (0.5%)
14	N	0.56	0/1704	1.05	12/2311 (0.5%)
All	All	0.50	0/48414	1.02	270/65598 (0.4%)

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
14	2	0	1
14	N	0	1
All	All	0	2

There are no bond length outliers.

The worst 5 of 270 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	L	106	LYS	N-CA-C	-12.24	98.77	112.72
12	Z	106	LYS	N-CA-C	-12.02	99.01	112.72
9	W	105	VAL	N-CA-C	-10.99	97.22	112.50
9	I	105	VAL	N-CA-C	-10.90	97.35	112.50
9	W	187	ARG	CA-C-N	-9.99	108.39	119.98

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
14	2	30	TYR	Sidechain
14	N	30	TYR	Sidechain

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	1842	0	1803	107	0
1	O	1842	0	1803	113	0
2	B	1707	0	1591	103	0
2	P	1707	0	1591	110	0
3	C	1902	0	1835	150	0
3	Q	1902	0	1835	148	0
4	D	1665	0	1433	110	0
4	R	1665	0	1433	112	0
5	E	1763	0	1708	89	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	S	1763	0	1708	86	0
6	F	1850	0	1822	106	0
6	T	1850	0	1822	98	0
7	G	1885	0	1843	94	0
7	U	1885	0	1843	89	0
8	H	1509	0	1473	66	0
8	V	1509	0	1473	60	0
9	I	1645	0	1649	114	0
9	W	1645	0	1649	104	0
10	J	1585	0	1600	118	0
10	X	1585	0	1600	112	0
11	K	1570	0	1546	107	0
11	Y	1570	0	1546	104	0
12	L	1548	0	1499	81	0
12	Z	1548	0	1499	86	0
13	1	1639	0	1609	85	0
13	M	1639	0	1609	72	0
14	2	1671	0	1625	84	0
14	N	1671	0	1625	86	0
15	1	2	0	0	0	0
15	A	1	0	0	0	0
15	B	1	0	0	0	0
15	C	1	0	0	0	0
15	D	1	0	0	0	0
15	G	3	0	0	0	0
15	I	1	0	0	0	0
15	J	4	0	0	0	0
15	K	1	0	0	0	0
15	M	2	0	0	0	0
15	O	1	0	0	0	0
15	P	1	0	0	0	0
15	Q	1	0	0	0	0
15	R	1	0	0	0	0
15	U	3	0	0	0	0
15	W	1	0	0	0	0
15	X	4	0	0	0	0
15	Y	1	0	0	0	0
16	1	4	0	0	1	0
16	2	8	0	0	1	0
16	A	2	0	0	0	0
16	B	3	0	0	0	0
16	C	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	F	6	0	0	1	0
16	G	4	0	0	1	0
16	H	7	0	0	0	0
16	I	6	0	0	2	0
16	J	1	0	0	0	0
16	K	6	0	0	0	0
16	L	8	0	0	0	0
16	M	10	0	0	0	0
16	N	9	0	0	4	0
16	O	7	0	0	1	0
16	P	6	0	0	1	0
16	Q	3	0	0	1	0
16	R	3	0	0	0	0
16	S	1	0	0	0	0
16	T	7	0	0	1	0
16	U	9	0	0	0	0
16	V	15	0	0	0	0
16	W	9	0	0	0	0
16	X	17	0	0	0	0
16	Y	3	0	0	1	0
16	Z	8	0	0	0	0
All	All	47757	0	46072	2569	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 27.

The worst 5 of 2569 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:145:ARG:HE	12:Z:158:ARG:HD2	1.01	1.14
3:Q:180:LYS:H	3:Q:180:LYS:HD3	1.10	1.11
12:L:158:ARG:HD2	11:Y:145:ARG:HE	1.10	1.08
3:C:180:LYS:HD3	3:C:180:LYS:H	1.10	1.07
4:D:57:ARG:HA	4:D:60:ARG:HE	1.18	1.06

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	242/246 (98%)	220 (91%)	19 (8%)	3 (1%)	10	20
1	O	242/246 (98%)	220 (91%)	19 (8%)	3 (1%)	10	20
2	B	231/233 (99%)	185 (80%)	30 (13%)	16 (7%)	1	1
2	P	231/233 (99%)	188 (81%)	28 (12%)	15 (6%)	1	1
3	C	248/261 (95%)	201 (81%)	34 (14%)	13 (5%)	1	2
3	Q	248/261 (95%)	202 (82%)	33 (13%)	13 (5%)	1	2
4	D	241/248 (97%)	192 (80%)	33 (14%)	16 (7%)	1	1
4	R	241/248 (97%)	191 (79%)	34 (14%)	16 (7%)	1	1
5	E	232/241 (96%)	205 (88%)	24 (10%)	3 (1%)	9	18
5	S	232/241 (96%)	205 (88%)	24 (10%)	3 (1%)	9	18
6	F	236/263 (90%)	214 (91%)	16 (7%)	6 (2%)	4	8
6	T	236/263 (90%)	214 (91%)	17 (7%)	5 (2%)	5	11
7	G	243/254 (96%)	223 (92%)	14 (6%)	6 (2%)	4	8
7	U	243/254 (96%)	221 (91%)	16 (7%)	6 (2%)	4	8
8	H	200/205 (98%)	188 (94%)	9 (4%)	3 (2%)	8	15
8	V	200/205 (98%)	188 (94%)	9 (4%)	3 (2%)	8	15
9	I	218/234 (93%)	193 (88%)	21 (10%)	4 (2%)	6	13
9	W	218/234 (93%)	193 (88%)	21 (10%)	4 (2%)	6	13
10	J	202/205 (98%)	180 (89%)	18 (9%)	4 (2%)	6	11
10	X	202/205 (98%)	180 (89%)	18 (9%)	4 (2%)	6	11
11	K	197/201 (98%)	174 (88%)	20 (10%)	3 (2%)	8	15
11	Y	197/201 (98%)	174 (88%)	20 (10%)	3 (2%)	8	15
12	L	199/204 (98%)	180 (90%)	17 (8%)	2 (1%)	12	24
12	Z	199/204 (98%)	181 (91%)	16 (8%)	2 (1%)	12	24
13	1	211/213 (99%)	191 (90%)	19 (9%)	1 (0%)	24	43

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	M	211/213 (99%)	192 (91%)	18 (8%)	1 (0%)	24	43
14	2	215/219 (98%)	195 (91%)	16 (7%)	4 (2%)	6	12
14	N	215/219 (98%)	196 (91%)	15 (7%)	4 (2%)	6	12
All	All	6230/6454 (96%)	5486 (88%)	578 (9%)	166 (3%)	4	7

5 of 166 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	40	ALA
2	B	52	LYS
2	B	54	ILE
2	B	60	SER
2	B	179	GLU

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	192/210 (91%)	186 (97%)	6 (3%)	35	59
1	O	192/210 (91%)	186 (97%)	6 (3%)	35	59
2	B	163/190 (86%)	152 (93%)	11 (7%)	15	28
2	P	163/190 (86%)	152 (93%)	11 (7%)	15	28
3	C	191/221 (86%)	181 (95%)	10 (5%)	21	39
3	Q	191/221 (86%)	181 (95%)	10 (5%)	21	39
4	D	136/211 (64%)	127 (93%)	9 (7%)	15	29
4	R	136/211 (64%)	128 (94%)	8 (6%)	18	33
5	E	190/204 (93%)	183 (96%)	7 (4%)	30	54
5	S	190/204 (93%)	183 (96%)	7 (4%)	30	54
6	F	198/224 (88%)	192 (97%)	6 (3%)	36	60
6	T	198/224 (88%)	191 (96%)	7 (4%)	32	56
7	G	195/211 (92%)	186 (95%)	9 (5%)	24	45

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	U	195/211 (92%)	186 (95%)	9 (5%)	24	45
8	H	155/159 (98%)	149 (96%)	6 (4%)	28	51
8	V	155/159 (98%)	149 (96%)	6 (4%)	28	51
9	I	177/195 (91%)	170 (96%)	7 (4%)	28	50
9	W	177/195 (91%)	170 (96%)	7 (4%)	28	50
10	J	172/174 (99%)	162 (94%)	10 (6%)	18	34
10	X	172/174 (99%)	162 (94%)	10 (6%)	18	34
11	K	164/171 (96%)	156 (95%)	8 (5%)	22	43
11	Y	164/171 (96%)	156 (95%)	8 (5%)	22	43
12	L	153/159 (96%)	146 (95%)	7 (5%)	24	45
12	Z	153/159 (96%)	146 (95%)	7 (5%)	24	45
13	1	173/178 (97%)	167 (96%)	6 (4%)	32	56
13	M	173/178 (97%)	167 (96%)	6 (4%)	32	56
14	2	174/181 (96%)	170 (98%)	4 (2%)	44	66
14	N	174/181 (96%)	170 (98%)	4 (2%)	44	66
All	All	4866/5376 (90%)	4654 (96%)	212 (4%)	25	47

5 of 212 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	P	132	SER
5	S	146	VAL
12	Z	180	ARG
2	P	155	PHE
3	Q	187	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 185 such sidechains are listed below:

Mol	Chain	Res	Type
3	Q	166	ASN
7	U	22	GLN
3	Q	235	GLN
5	S	211	ASN
8	V	158	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 30 ligands modelled in this entry, 30 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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, 95th 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 ²)	Q<0.9
1	A	244/246 (99%)	1.36	58 (23%) 2 1	56, 89, 120, 135	0
1	O	244/246 (99%)	0.20	6 (2%) 58 56	38, 56, 81, 100	0
2	B	233/233 (100%)	1.51	59 (25%) 1 1	62, 97, 133, 142	0
2	P	233/233 (100%)	0.61	15 (6%) 25 25	36, 67, 105, 129	0
3	C	250/261 (95%)	1.52	67 (26%) 1 1	59, 103, 142, 148	0
3	Q	250/261 (95%)	0.80	15 (6%) 27 28	37, 70, 123, 141	0
4	D	243/248 (97%)	1.23	39 (16%) 5 4	54, 93, 146, 163	0
4	R	243/248 (97%)	1.13	51 (20%) 2 2	40, 82, 134, 157	0
5	E	234/241 (97%)	0.40	9 (3%) 44 41	39, 64, 94, 110	0
5	S	234/241 (97%)	0.73	18 (7%) 19 19	39, 74, 102, 132	0
6	F	238/263 (90%)	0.35	5 (2%) 63 61	42, 63, 91, 124	0
6	T	238/263 (90%)	0.34	10 (4%) 40 39	37, 58, 95, 135	0
7	G	245/254 (96%)	0.84	19 (7%) 19 19	49, 74, 104, 118	0
7	U	245/254 (96%)	0.19	9 (3%) 45 42	35, 53, 89, 126	0
8	H	202/205 (98%)	0.47	2 (0%) 79 79	35, 60, 78, 94	0
8	V	202/205 (98%)	0.17	4 (1%) 65 63	33, 49, 70, 102	0
9	I	220/234 (94%)	1.01	20 (9%) 15 14	49, 71, 100, 115	0
9	W	220/234 (94%)	0.17	0 100 100	30, 53, 81, 99	0
10	J	204/205 (99%)	1.20	34 (16%) 4 4	49, 79, 101, 111	0
10	X	204/205 (99%)	0.33	7 (3%) 48 46	36, 52, 78, 97	0
11	K	199/201 (99%)	0.86	15 (7%) 20 20	49, 69, 93, 110	0
11	Y	199/201 (99%)	0.43	6 (3%) 52 50	36, 56, 80, 113	0
12	L	201/204 (98%)	0.24	5 (2%) 58 56	35, 53, 75, 108	0
12	Z	201/204 (98%)	0.72	10 (4%) 34 34	45, 65, 85, 106	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	1	213/213 (100%)	0.73	17 (7%) 18 18	40, 70, 97, 112	0
13	M	213/213 (100%)	0.06	1 (0%) 87 87	31, 50, 73, 97	0
14	2	217/219 (99%)	0.33	4 (1%) 67 65	33, 55, 81, 109	0
14	N	217/219 (99%)	0.09	3 (1%) 73 73	33, 51, 70, 109	0
All	All	6286/6454 (97%)	0.65	508 (8%) 18 18	30, 66, 115, 163	0

The worst 5 of 508 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	1	ALA	6.5
13	1	166	LEU	5.8
3	C	171	ALA	5.4
2	P	1	ALA	5.3
2	P	233	ALA	4.9

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 oligosaccharides 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, 95th 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 ²)	Q<0.9
15	MG	A	301	1/1	0.64	0.19	83,83,83,83	0
15	MG	K	313	1/1	0.67	0.19	77,77,77,77	0
15	MG	D	309	1/1	0.70	0.23	87,87,87,87	0
15	MG	I	306	1/1	0.76	0.24	87,87,87,87	0
15	MG	G	319	1/1	0.77	0.13	66,66,66,66	0
15	MG	X	404	1/1	0.77	0.24	70,70,70,70	0
15	MG	U	417	1/1	0.79	0.19	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
15	MG	Q	414	1/1	0.79	0.21	90,90,90,90	0
15	MG	1	418	1/1	0.82	0.20	90,90,90,90	0
15	MG	O	401	1/1	0.85	0.16	57,57,57,57	0
15	MG	M	318	1/1	0.86	0.11	81,81,81,81	0
15	MG	C	314	1/1	0.86	0.12	76,76,76,76	0
15	MG	G	317	1/1	0.88	0.15	85,85,85,85	0
15	MG	J	304	1/1	0.89	0.08	56,56,56,56	0
15	MG	U	419	1/1	0.89	0.14	70,70,70,70	0
15	MG	J	315	1/1	0.89	0.10	69,69,69,69	0
15	MG	G	311	1/1	0.89	0.18	97,97,97,97	0
15	MG	B	316	1/1	0.90	0.09	84,84,84,84	0
15	MG	W	406	1/1	0.90	0.09	59,59,59,59	0
15	MG	X	415	1/1	0.91	0.11	59,59,59,59	0
15	MG	Y	413	1/1	0.91	0.17	51,51,51,51	0
15	MG	J	407	1/1	0.91	0.08	70,70,70,70	0
15	MG	1	410	1/1	0.92	0.09	66,66,66,66	0
15	MG	J	320	1/1	0.92	0.14	112,112,112,112	0
15	MG	X	420	1/1	0.93	0.18	77,77,77,77	0
15	MG	P	416	1/1	0.93	0.08	72,72,72,72	0
15	MG	M	310	1/1	0.94	0.07	67,67,67,67	0
15	MG	R	409	1/1	0.94	0.10	59,59,59,59	0
15	MG	U	411	1/1	0.94	0.15	76,76,76,76	0
15	MG	X	307	1/1	0.96	0.08	39,39,39,39	0

6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.