wwPDB EM Map/Model Validation Report (i)

Sep 12, 2016 – 07:26 PM EDT

PDB ID	:	5L4G
EMDB ID:	:	EMD-4002
Title	:	The human 26S proteasome at 3.9 A
Authors	:	Schweitzer, A.; Aufderheide, A.; Rudack, T.; Beck, F.
Deposited on	:	2016-05-25
Resolution	:	4.02 Å(reported)

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could
stem from errors in the original structure(s) used in the fitting.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/EMValidationReportHelp

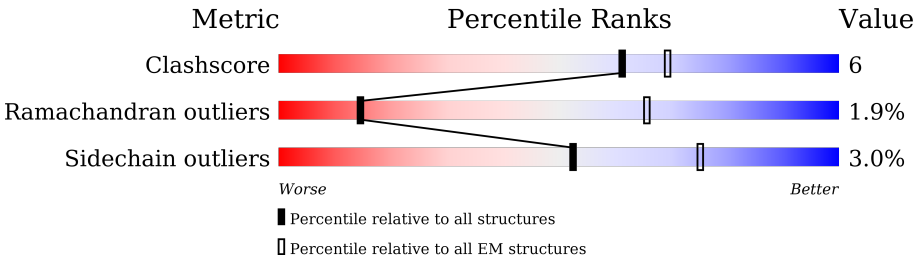
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027939

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 4.02 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)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for >=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 <=5%

Mol	Chain	Length	Quality of chain
1	A	246	86% 13% •
1	N	246	85% 14% •
2	B	234	81% 15% •
2	O	234	83% 15% •
3	C	261	89% 6% •
3	P	261	85% 9% • •
4	D	248	86% 11% • •
4	Q	248	87% 11% •
5	E	241	85% 11% • •

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Mol	Chain	Length	Quality of chain
5	R	241	85% 11% •
6	F	263	75% 15% 10%
6	S	263	79% 11% 10%
7	G	255	82% 13% 5%
7	T	255	87% 7% 5%
8	1	241	75% 12% • 12%
8	U	241	72% 15% • 12%
9	2	201	88% 9% ••
9	V	201	88% 10% ••
10	3	205	83% 15% •
10	W	205	93% 6%
11	4	264	72% 11% 18%
11	X	264	75% 6% • 18%
12	5	263	63% 13% 24%
12	Y	263	63% 11% • 24%
13	6	239	74% 8% 17%
13	Z	239	72% 12% 16%
14	7	277	69% 9% • 21%
14	8	277	70% 8% • 21%
15	H	433	65% 24% • 9%
16	I	440	66% 19% • 14%
17	K	418	75% 17% • 6%
18	L	389	80% 17% •
19	M	439	74% 18% • 5%
20	J	406	73% 21% • •

2 Entry composition

There are 23 unique types of molecules in this entry. The entry contains 135560 atoms, of which 67868 are hydrogens and 0 are deuteriums.

In the tables below, 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-6.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	N	244	Total	C	H	N	O	S	0	0
			3814	1206	1911	320	364	13		
1	A	244	Total	C	H	N	O	S	0	0
			3814	1206	1911	320	364	13		

- Molecule 2 is a protein called Proteasome subunit alpha type-2.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	O	233	Total	C	H	N	O	S	0	0
			3630	1161	1812	308	343	6		
2	B	233	Total	C	H	N	O	S	0	0
			3630	1161	1812	308	343	6		

- Molecule 3 is a protein called Proteasome subunit alpha type-4.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	P	250	Total	C	H	N	O	S	0	0
			3963	1245	1992	339	377	10		
3	C	250	Total	C	H	N	O	S	0	0
			3963	1245	1992	339	377	10		

- Molecule 4 is a protein called Proteasome subunit alpha type-7.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	Q	243	Total	C	H	N	O	S	0	0
			3875	1206	1952	342	370	5		
4	D	243	Total	C	H	N	O	S	0	0
			3875	1206	1952	342	370	5		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
5	R	234	Total	C	H	N	O	S	0	0
			3563	1125	1773	295	359	11		
5	E	234	Total	C	H	N	O	S	0	0
			3563	1125	1773	295	359	11		

- Molecule 6 is a protein called Proteasome subunit alpha type-1.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	S	238	Total	C	H	N	O	S	0	0
			3733	1172	1860	337	353	11		
6	F	238	Total	C	H	N	O	S	0	0
			3733	1172	1860	337	353	11		

- Molecule 7 is a protein called Proteasome subunit alpha type-3.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	T	242	Total	C	H	N	O	S	0	0
			3771	1200	1877	323	360	11		
7	G	241	Total	C	H	N	O	S	0	0
			3764	1198	1874	322	359	11		

- Molecule 8 is a protein called Proteasome subunit beta type-1.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	U	213	Total	C	H	N	O	S	0	0
			3308	1047	1654	284	313	10		
8	1	213	Total	C	H	N	O	S	0	0
			3308	1047	1654	284	313	10		

- Molecule 9 is a protein called Proteasome subunit beta type-2.

Mol	Chain	Residues	Atoms						AltConf	Trace
9	V	199	Total	C	H	N	O	S	0	0
			3197	1022	1601	272	293	9		
9	2	199	Total	C	H	N	O	S	0	0
			3197	1022	1601	272	293	9		

- Molecule 10 is a protein called Proteasome subunit beta type-3.

Mol	Chain	Residues	Atoms						AltConf	Trace
10	W	204	Total	C	H	N	O	S	0	0
			3200	1013	1609	265	294	19		

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Mol	Chain	Residues	Atoms						AltConf	Trace
10	3	204	Total	C	H	N	O	S	0	0
			3200	1013	1609	265	294	19		

- Molecule 11 is a protein called Proteasome subunit beta type-4.

Mol	Chain	Residues	Atoms						AltConf	Trace
11	X	217	Total	C	H	N	O	S	0	0
			3358	1066	1667	292	321	12		
11	4	217	Total	C	H	N	O	S	0	0
			3358	1066	1667	292	321	12		

- Molecule 12 is a protein called Proteasome subunit beta type-5.

Mol	Chain	Residues	Atoms						AltConf	Trace
12	Y	201	Total	C	H	N	O	S	0	0
			3080	982	1521	274	294	9		
12	5	201	Total	C	H	N	O	S	0	0
			3080	982	1521	274	294	9		

- Molecule 13 is a protein called Proteasome subunit beta type-6.

Mol	Chain	Residues	Atoms						AltConf	Trace
13	Z	200	Total	C	H	N	O	S	0	0
			2966	939	1467	256	292	12		
13	6	199	Total	C	H	N	O	S	0	0
			2956	936	1462	255	291	12		

- Molecule 14 is a protein called Proteasome subunit beta type-7.

Mol	Chain	Residues	Atoms						AltConf	Trace
14	8	220	Total	C	H	N	O	S	0	0
			3338	1044	1679	283	320	12		
14	7	220	Total	C	H	N	O	S	0	0
			3338	1044	1679	283	320	12		

- Molecule 15 is a protein called 26S protease regulatory subunit 7.

Mol	Chain	Residues	Atoms						AltConf	Trace
15	H	396	Total	C	H	N	O	S	0	0
			6283	1961	3167	549	588	18		

- Molecule 16 is a protein called 26S protease regulatory subunit 4.

Mol	Chain	Residues	Atoms						AltConf	Trace
16	I	379	Total	C	H	N	O	S	0	0
			6043	1880	3050	510	588	15		

- Molecule 17 is a protein called 26S protease regulatory subunit 6B.

Mol	Chain	Residues	Atoms						AltConf	Trace
17	K	393	Total	C	H	N	O	S	0	0
			6302	1986	3164	537	602	13		

- Molecule 18 is a protein called 26S protease regulatory subunit 10B.

Mol	Chain	Residues	Atoms						AltConf	Trace
18	L	389	Total	C	H	N	O	S	0	0
			6271	1947	3173	552	582	17		

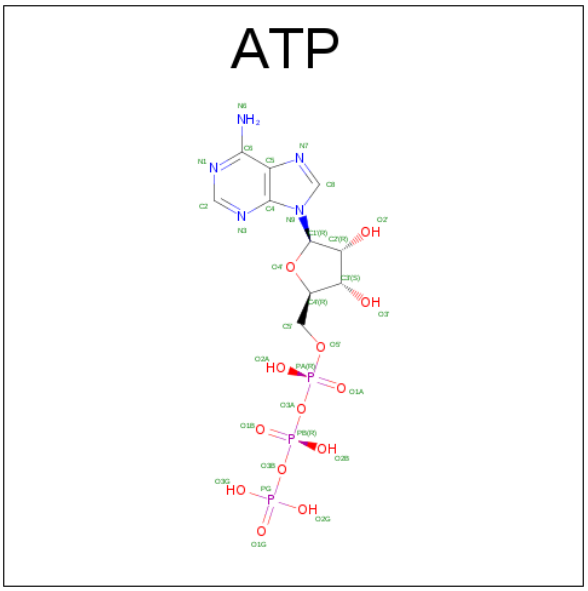
- Molecule 19 is a protein called 26S protease regulatory subunit 6A.

Mol	Chain	Residues	Atoms						AltConf	Trace
19	M	415	Total	C	H	N	O	S	0	0
			6575	2039	3322	561	635	18		

- Molecule 20 is a protein called 26S protease regulatory subunit 8.

Mol	Chain	Residues	Atoms						AltConf	Trace
20	J	391	Total	C	H	N	O	S	0	0
			6252	1928	3178	549	579	18		

- Molecule 21 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).

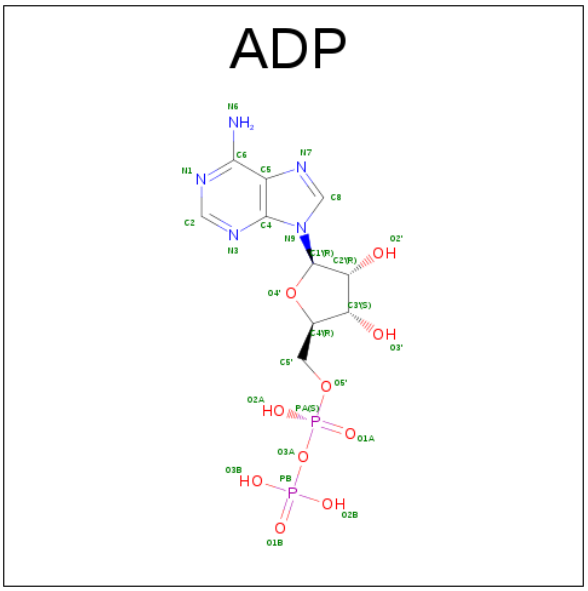


Mol	Chain	Residues	Atoms						AltConf
21	H	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	
21	I	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	
21	K	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	
21	L	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	
21	M	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	

- Molecule 22 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
22	H	1	Total	Mg	0
			1	1	
22	I	1	Total	Mg	0
			1	1	
22	L	1	Total	Mg	0
			1	1	
22	K	1	Total	Mg	0
			1	1	
22	M	1	Total	Mg	0
			1	1	

- Molecule 23 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



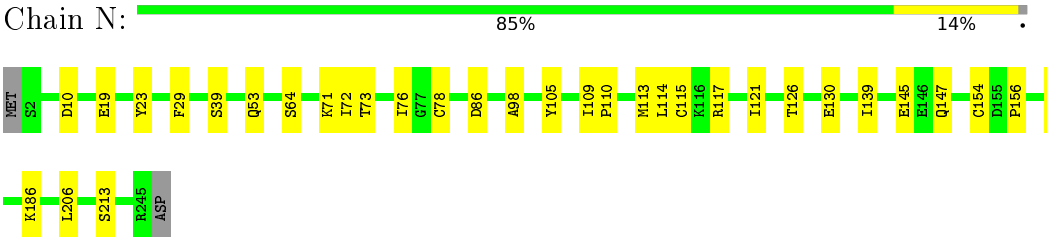
Mol	Chain	Residues	Atoms						AltConf
23	J	1	Total	C	H	N	O	P	0
			39	10	12	5	10	2	

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 errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

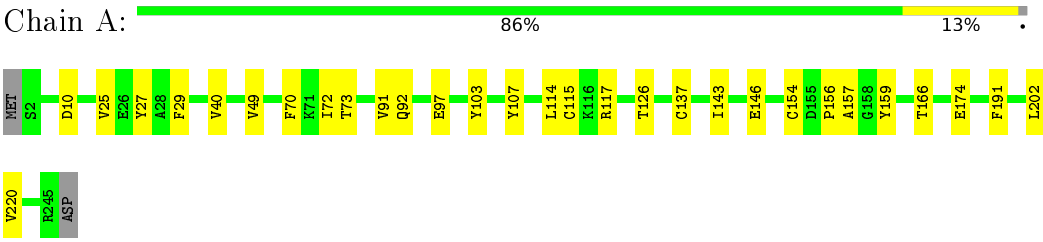
- Molecule 1: Proteasome subunit alpha type-6

Chain N:



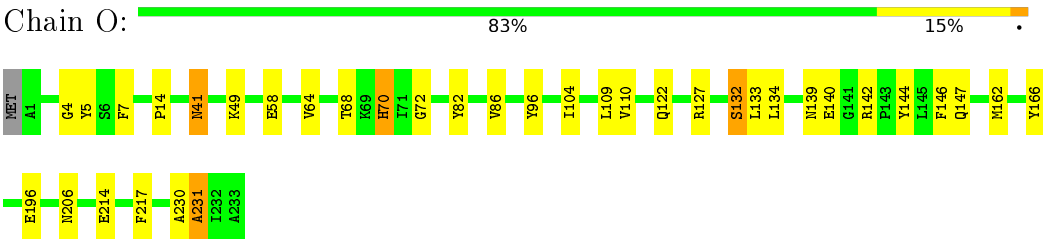
- Molecule 1: Proteasome subunit alpha type-6

Chain A:



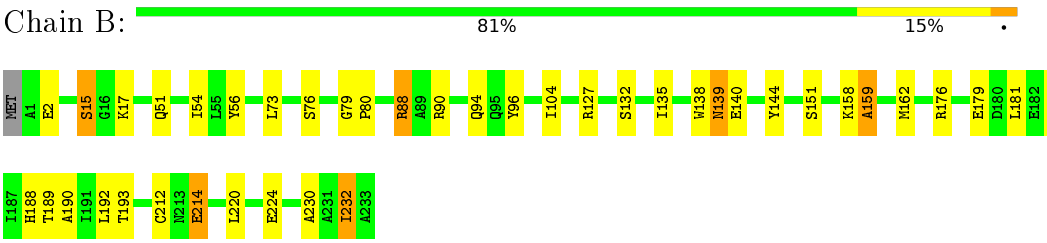
- Molecule 2: Proteasome subunit alpha type-2

Chain O:



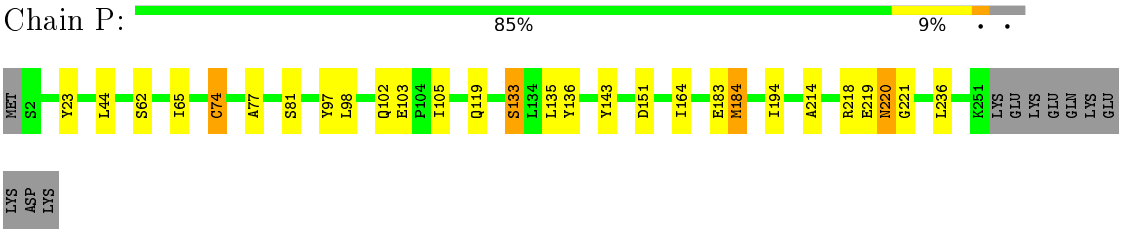
- Molecule 2: Proteasome subunit alpha type-2

Chain B:



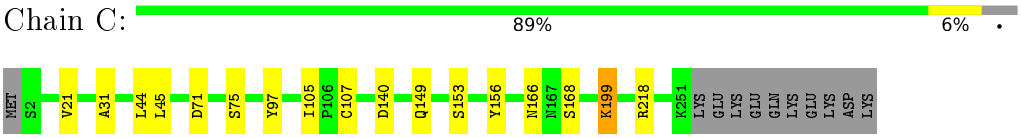
- Molecule 3: Proteasome subunit alpha type-4

Chain P:



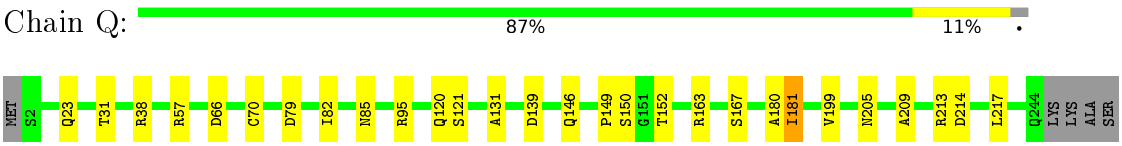
- Molecule 3: Proteasome subunit alpha type-4

Chain C:



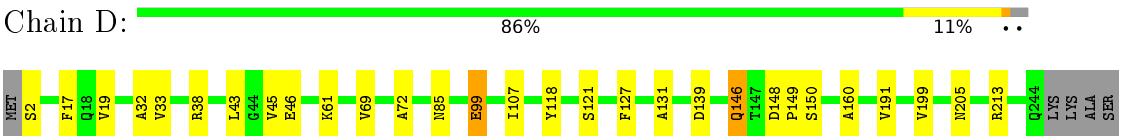
- Molecule 4: Proteasome subunit alpha type-7

Chain Q:



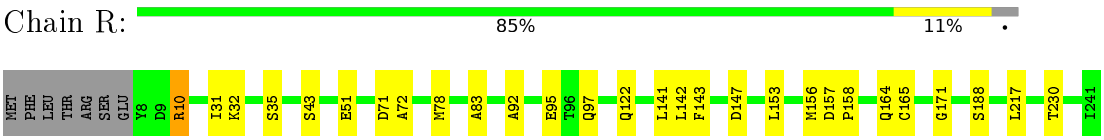
- Molecule 4: Proteasome subunit alpha type-7

Chain D:



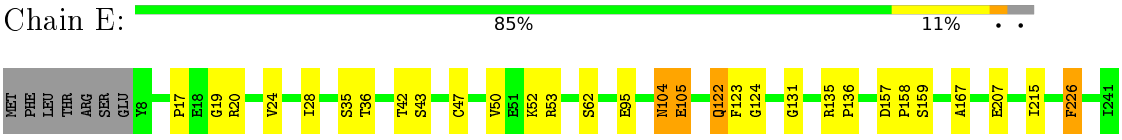
- Molecule 5: Proteasome subunit alpha type-5

Chain R:



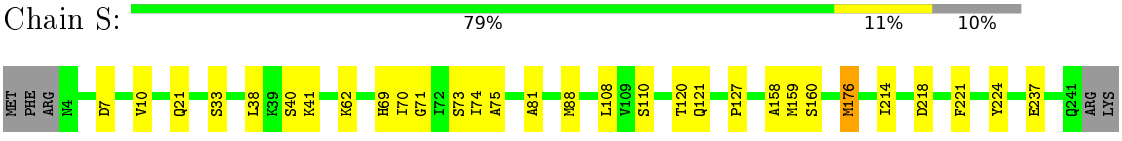
- Molecule 5: Proteasome subunit alpha type-5

Chain E:



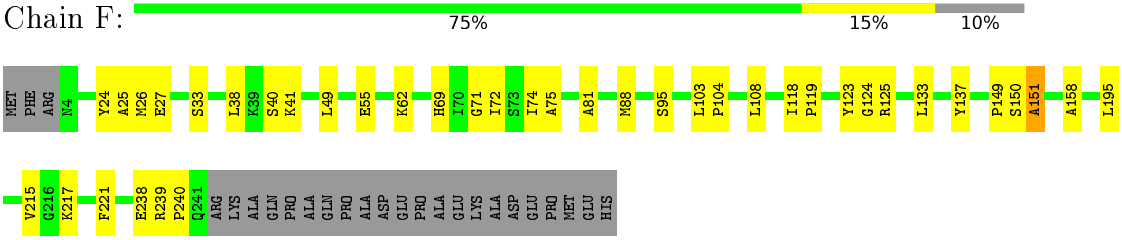
- Molecule 6: Proteasome subunit alpha type-1

Chain S:



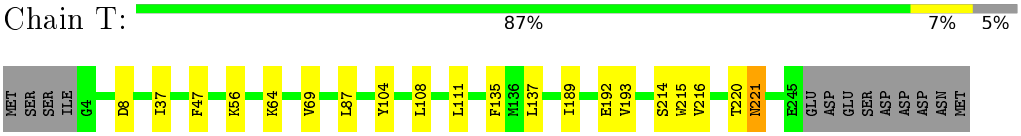
- Molecule 6: Proteasome subunit alpha type-1

Chain F:



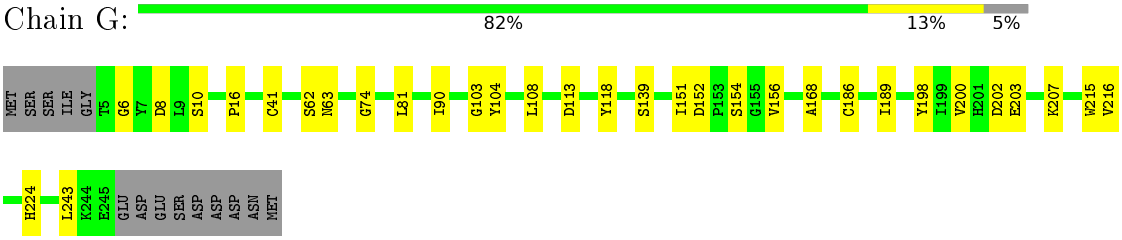
- Molecule 7: Proteasome subunit alpha type-3

Chain T:



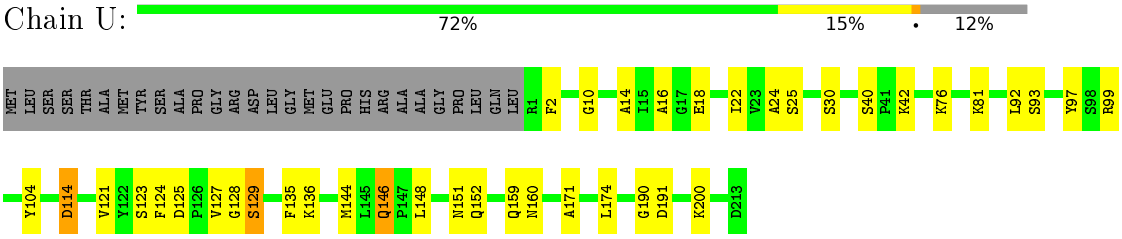
- Molecule 7: Proteasome subunit alpha type-3

Chain G:



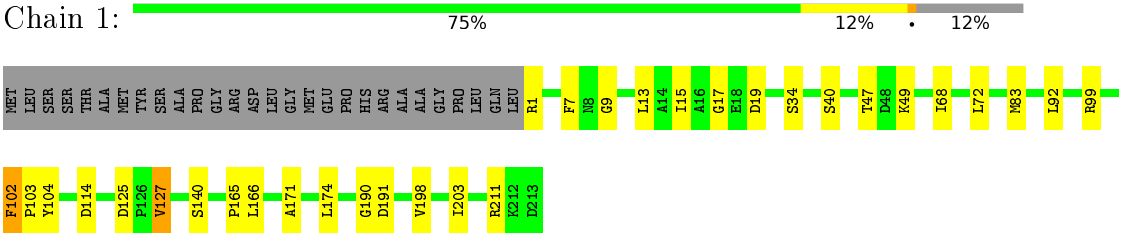
- Molecule 8: Proteasome subunit beta type-1

Chain U:



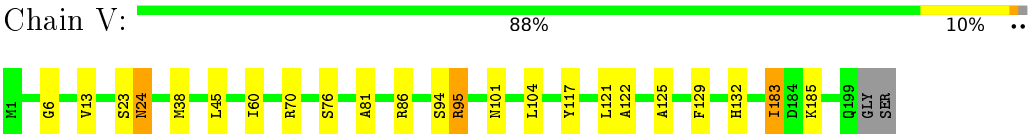
- Molecule 8: Proteasome subunit beta type-1

Chain 1:



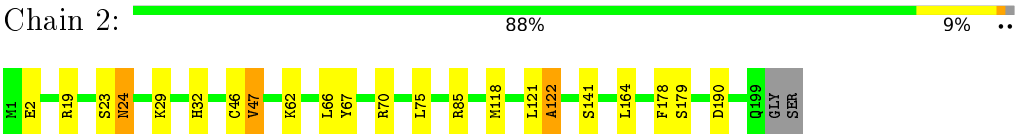
- Molecule 9: Proteasome subunit beta type-2

Chain V:



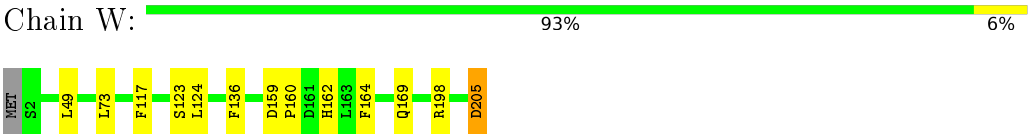
• Molecule 9: Proteasome subunit beta type-2

Chain 2:



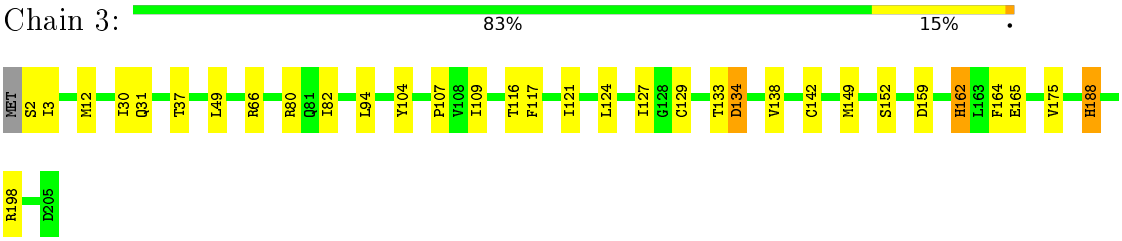
• Molecule 10: Proteasome subunit beta type-3

Chain W:



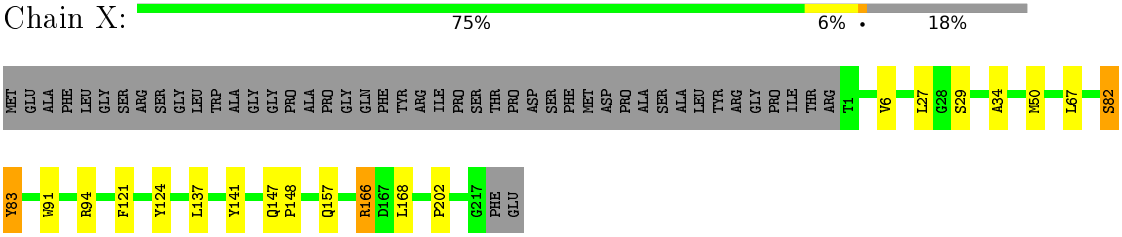
• Molecule 10: Proteasome subunit beta type-3

Chain 3:



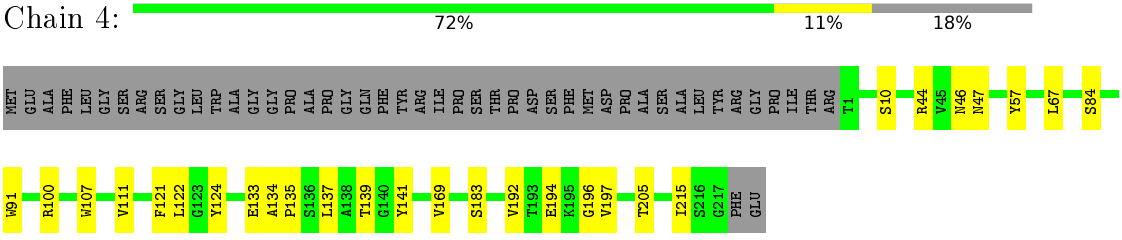
• Molecule 11: Proteasome subunit beta type-4

Chain X:



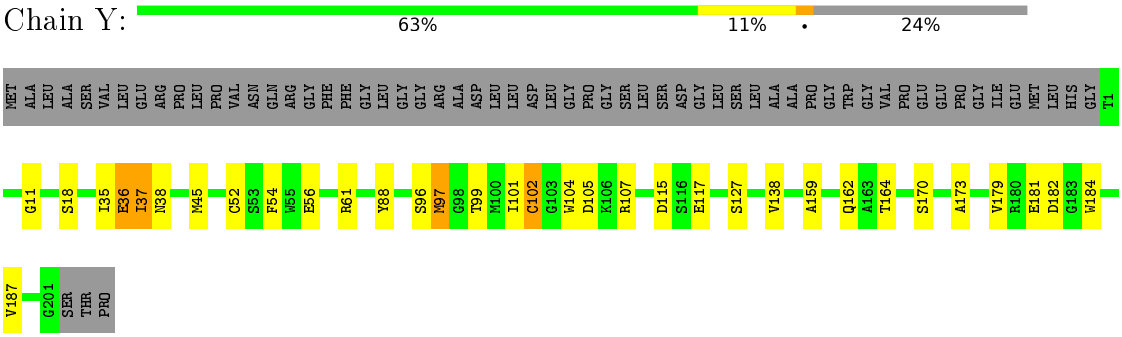
• Molecule 11: Proteasome subunit beta type-4

Chain 4:



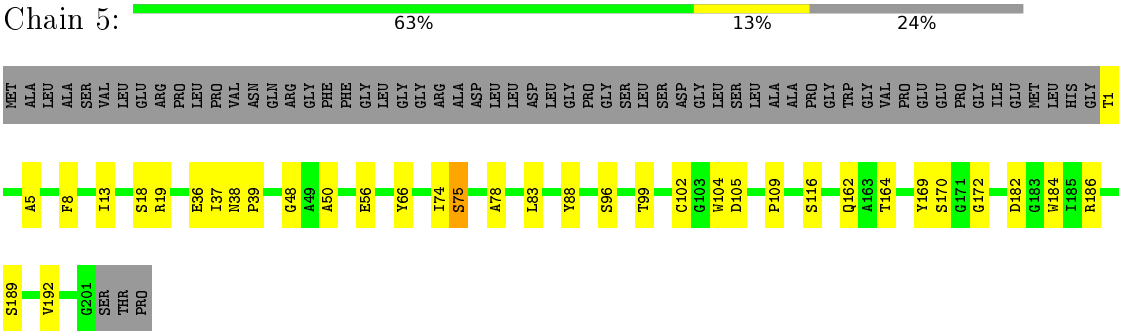
• Molecule 12: Proteasome subunit beta type-5

Chain Y:



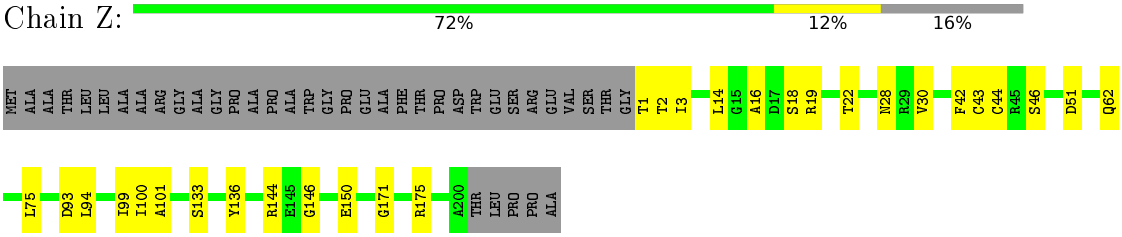
- Molecule 12: Proteasome subunit beta type-5

Chain 5:



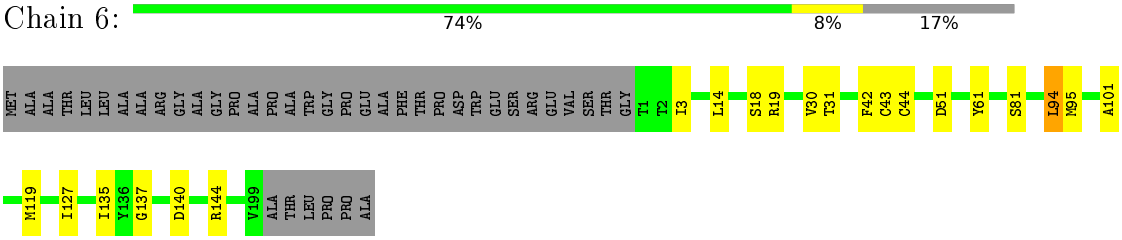
- Molecule 13: Proteasome subunit beta type-6

Chain Z:



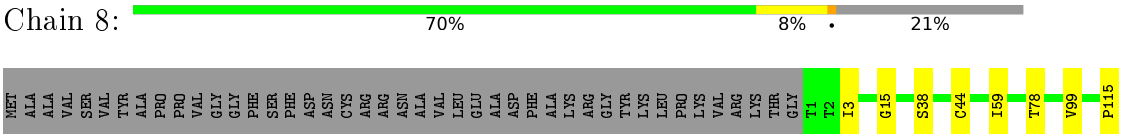
- Molecule 13: Proteasome subunit beta type-6

Chain 6:



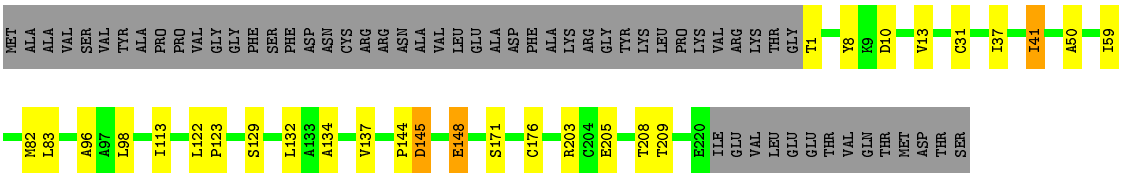
- Molecule 14: Proteasome subunit beta type-7

Chain 8:



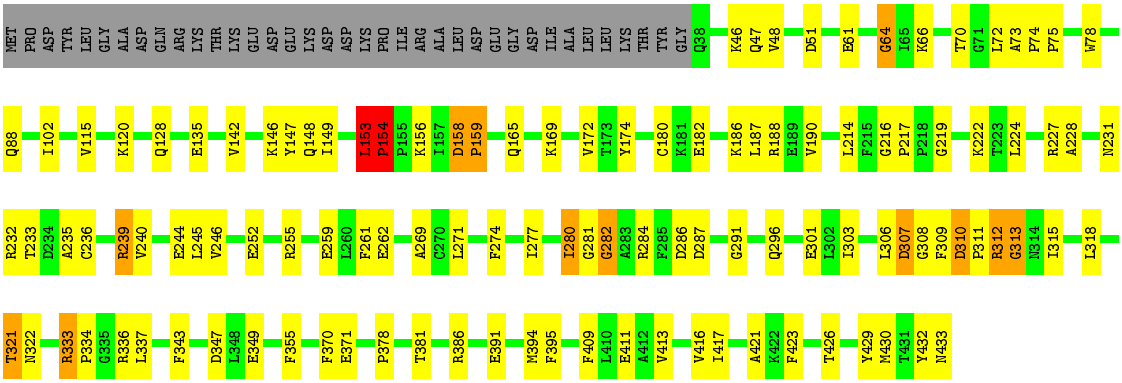
• Molecule 14: Proteasome subunit beta type-7

Chain 7:



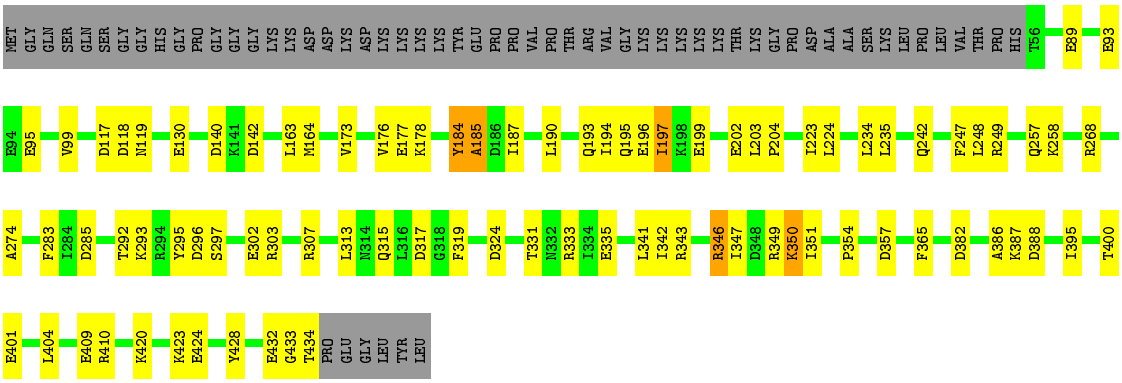
• Molecule 15: 26S protease regulatory subunit 7

Chain H:



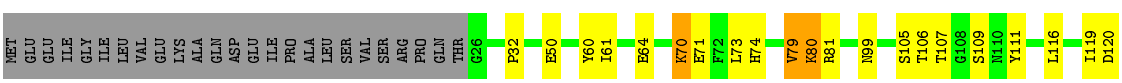
• Molecule 16: 26S protease regulatory subunit 4

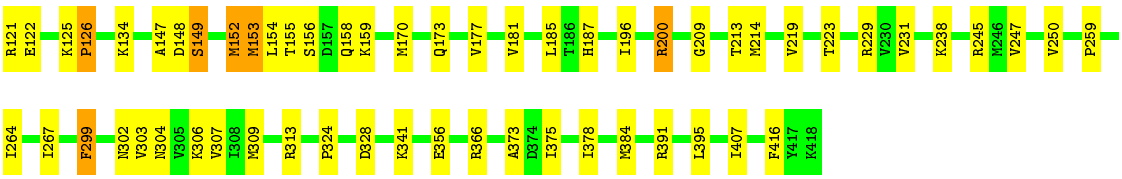
Chain I:



• Molecule 17: 26S protease regulatory subunit 6B

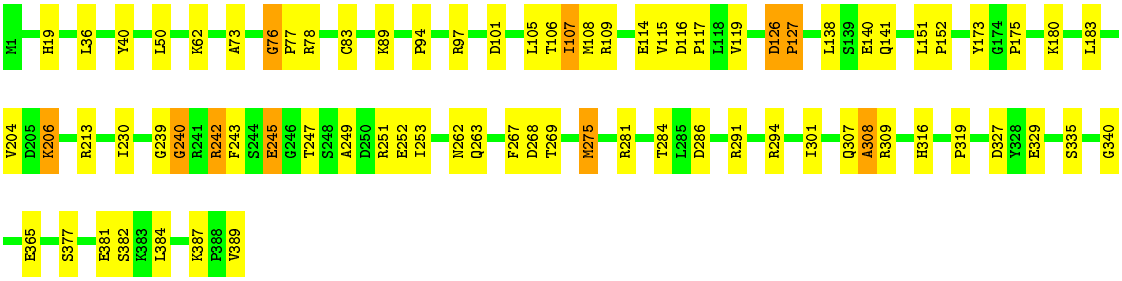
Chain K:





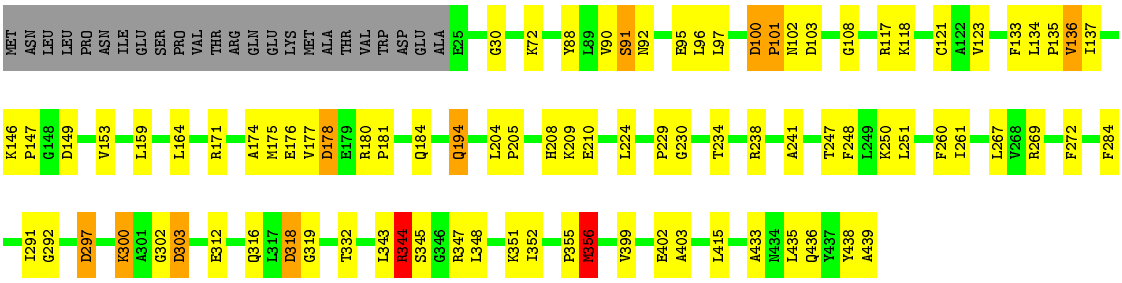
- Molecule 18: 26S protease regulatory subunit 10B

Chain L:



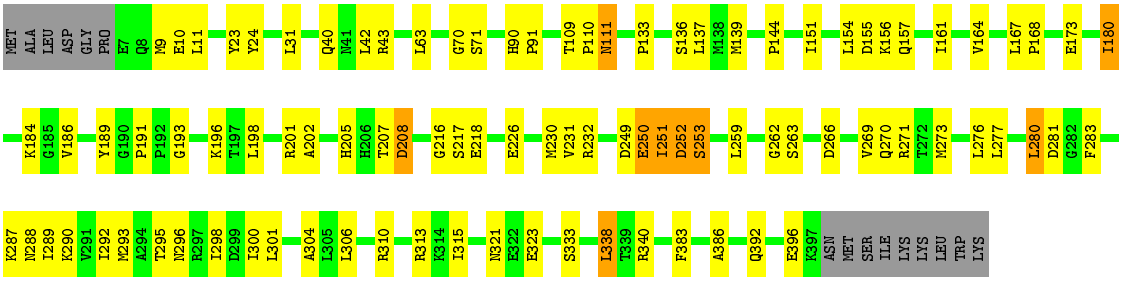
- Molecule 19: 26S protease regulatory subunit 6A

Chain M:



- Molecule 20: 26S protease regulatory subunit 8

Chain J:



4 Experimental information (i)

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	461402	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	Not provided	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	Not provided	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ATP, ADP

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	#$\|Z\|>2$	RMSZ	#$\|Z\|>2$
1	A	0.43	0/1937	0.55	0/2617
1	N	0.38	0/1937	0.56	0/2617
10	3	0.42	1/1620 (0.1%)	0.57	0/2184
10	W	0.40	0/1620	0.58	0/2184
11	4	0.42	0/1724	0.61	0/2333
11	X	0.40	0/1724	0.59	0/2333
12	5	0.42	0/1590	0.59	0/2147
12	Y	0.41	0/1590	0.60	0/2147
13	6	0.40	0/1520	0.56	0/2057
13	Z	0.39	0/1525	0.60	0/2064
14	7	0.36	0/1686	0.58	0/2282
14	8	0.35	0/1686	0.58	0/2282
15	H	0.38	0/3168	0.61	2/4277 (0.0%)
16	I	0.35	0/3034	0.58	0/4089
17	K	0.37	0/3191	0.53	0/4306
18	L	0.38	0/3146	0.56	0/4233
19	M	0.38	0/3294	0.54	0/4437
2	B	0.88	6/1857 (0.3%)	0.78	9/2514 (0.4%)
2	O	0.38	0/1857	0.54	0/2514
20	J	0.39	0/3113	0.56	0/4184
3	C	0.38	0/2001	0.56	0/2694
3	P	0.36	0/2001	0.56	0/2694
4	D	0.37	0/1949	0.55	0/2626
4	Q	0.34	0/1949	0.52	0/2626
5	E	0.38	0/1818	0.56	0/2455
5	R	0.37	0/1818	0.53	0/2455
6	F	0.36	0/1908	0.56	0/2579
6	S	0.34	0/1908	0.54	0/2579
7	G	0.38	0/1925	0.55	0/2592
7	T	0.37	0/1929	0.53	0/2597
8	1	0.41	0/1684	0.58	0/2268
8	U	0.38	0/1684	0.59	0/2268

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >2	RMSZ	#|Z| >2
9	2	0.43	0/1629	0.58	0/2203
9	V	0.42	0/1629	0.58	0/2203
All	All	0.41	7/68651 (0.0%)	0.57	11/92640 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
15	H	0	2
16	I	0	1
17	K	0	2
2	B	0	1
20	J	0	1
7	G	0	1
7	T	0	1
All	All	0	9

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	185	ASP	CB-CG	20.70	1.95	1.51
2	B	185	ASP	CA-CB	17.41	1.92	1.53
2	B	184	GLU	CB-CG	13.19	1.77	1.52
2	B	184	GLU	C-N	8.40	1.53	1.34
2	B	185	ASP	N-CA	7.22	1.60	1.46

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	185	ASP	N-CA-CB	12.31	132.76	110.60
2	B	184	GLU	C-N-CA	11.92	151.50	121.70
15	H	153	LEU	C-N-CD	-11.44	95.42	120.60
2	B	185	ASP	CB-CG-OD1	8.30	125.77	118.30
2	B	185	ASP	CB-CA-C	-8.00	94.41	110.40

There are no chirality outliers.

5 of 9 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	186	ALA	Peptide
7	G	215	TRP	Peptide
15	H	153	LEU	Peptide
15	H	321	THR	Peptide
7	T	215	TRP	Peptide

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	1903	1911	1911	17	0
1	N	1903	1911	1911	18	0
2	B	1818	1812	1814	46	0
2	O	1818	1812	1814	20	0
3	C	1971	1992	1992	7	0
3	P	1971	1992	1992	16	0
4	D	1923	1952	1952	15	0
4	Q	1923	1952	1952	12	0
5	E	1790	1773	1773	14	0
5	R	1790	1773	1773	13	0
6	F	1873	1860	1860	21	0
6	S	1873	1860	1860	12	0
7	G	1890	1874	1874	11	0
7	T	1894	1877	1877	9	0
8	1	1654	1654	1656	13	0
8	U	1654	1654	1656	23	0
9	2	1596	1601	1601	15	0
9	V	1596	1601	1601	14	0
10	3	1591	1609	1609	20	0
10	W	1591	1609	1609	7	0
11	4	1691	1667	1669	14	0
11	X	1691	1667	1669	9	0
12	5	1559	1521	1523	15	0
12	Y	1559	1521	1523	21	0
13	6	1494	1462	1464	10	0
13	Z	1499	1467	1469	14	0
14	7	1659	1679	1681	20	0
14	8	1659	1679	1681	12	0
15	H	3116	3167	3167	90	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	I	2993	3050	3050	63	0
17	K	3138	3164	3164	52	0
18	L	3098	3173	3173	52	0
19	M	3253	3322	3322	71	0
20	J	3074	3178	3178	73	0
21	H	31	12	12	2	0
21	I	31	12	12	0	0
21	K	31	12	12	5	0
21	L	31	12	12	1	0
21	M	31	12	12	4	0
22	H	1	0	0	0	0
22	I	1	0	0	0	0
22	K	1	0	0	0	0
22	L	1	0	0	0	0
22	M	1	0	0	0	0
23	J	27	12	12	2	0
All	All	67692	67868	67892	756	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

The worst 5 of 756 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:B:184:GLU:CG	2:B:184:GLU:CB	1.77	1.54
2:B:185:ASP:CA	2:B:185:ASP:CB	1.92	1.45
2:B:185:ASP:CG	2:B:185:ASP:CB	1.95	1.35
2:B:185:ASP:O	2:B:189:THR:N	1.81	1.14
17:K:70:LYS:O	17:K:73:LEU:N	1.97	0.96

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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%)	217 (90%)	23 (10%)	2 (1%)	24	69
1	N	242/246 (98%)	215 (89%)	25 (10%)	2 (1%)	24	69
2	B	231/234 (99%)	208 (90%)	20 (9%)	3 (1%)	15	61
2	O	231/234 (99%)	206 (89%)	21 (9%)	4 (2%)	11	56
3	C	248/261 (95%)	235 (95%)	13 (5%)	0	100	100
3	P	248/261 (95%)	230 (93%)	15 (6%)	3 (1%)	16	62
4	D	241/248 (97%)	221 (92%)	18 (8%)	2 (1%)	24	69
4	Q	241/248 (97%)	217 (90%)	20 (8%)	4 (2%)	11	56
5	E	232/241 (96%)	207 (89%)	17 (7%)	8 (3%)	5	43
5	R	232/241 (96%)	207 (89%)	22 (10%)	3 (1%)	15	61
6	F	236/263 (90%)	214 (91%)	17 (7%)	5 (2%)	9	52
6	S	236/263 (90%)	218 (92%)	14 (6%)	4 (2%)	11	56
7	G	239/255 (94%)	212 (89%)	24 (10%)	3 (1%)	15	61
7	T	240/255 (94%)	224 (93%)	13 (5%)	3 (1%)	15	61
8	1	211/241 (88%)	189 (90%)	17 (8%)	5 (2%)	7	50
8	U	211/241 (88%)	186 (88%)	22 (10%)	3 (1%)	14	59
9	2	197/201 (98%)	176 (89%)	18 (9%)	3 (2%)	13	58
9	V	197/201 (98%)	177 (90%)	17 (9%)	3 (2%)	13	58
10	3	202/205 (98%)	180 (89%)	21 (10%)	1 (0%)	34	76
10	W	202/205 (98%)	180 (89%)	20 (10%)	2 (1%)	19	65
11	4	215/264 (81%)	193 (90%)	21 (10%)	1 (0%)	34	76
11	X	215/264 (81%)	196 (91%)	15 (7%)	4 (2%)	10	54
12	5	199/263 (76%)	176 (88%)	19 (10%)	4 (2%)	9	54
12	Y	199/263 (76%)	178 (89%)	16 (8%)	5 (2%)	7	49
13	6	197/239 (82%)	177 (90%)	17 (9%)	3 (2%)	13	58
13	Z	198/239 (83%)	177 (89%)	19 (10%)	2 (1%)	19	65
14	7	218/277 (79%)	195 (89%)	21 (10%)	2 (1%)	21	67
14	8	218/277 (79%)	192 (88%)	24 (11%)	2 (1%)	21	67
15	H	394/433 (91%)	323 (82%)	51 (13%)	20 (5%)	2	31
16	I	377/440 (86%)	332 (88%)	41 (11%)	4 (1%)	17	64

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
17	K	391/418 (94%)	323 (83%)	53 (14%)	15 (4%)	4 39
18	L	387/389 (100%)	326 (84%)	45 (12%)	16 (4%)	3 37
19	M	413/439 (94%)	348 (84%)	50 (12%)	15 (4%)	4 41
20	J	389/406 (96%)	326 (84%)	52 (13%)	11 (3%)	6 47
All	All	8569/9401 (91%)	7581 (88%)	821 (10%)	167 (2%)	14 54

5 of 167 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	O	41	ASN
2	O	70	HIS
4	Q	120	GLN
7	T	64	LYS
8	U	2	PHE

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 PDB entries followed by that with respect to all EM entries.

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	208/210 (99%)	204 (98%)	4 (2%)	65 86
1	N	208/210 (99%)	202 (97%)	6 (3%)	50 79
2	B	190/191 (100%)	178 (94%)	12 (6%)	22 61
2	O	190/191 (100%)	184 (97%)	6 (3%)	46 78
3	C	210/221 (95%)	205 (98%)	5 (2%)	57 82
3	P	210/221 (95%)	205 (98%)	5 (2%)	57 82
4	D	207/211 (98%)	200 (97%)	7 (3%)	44 77
4	Q	207/211 (98%)	200 (97%)	7 (3%)	44 77
5	E	196/203 (97%)	189 (96%)	7 (4%)	42 76
5	R	196/203 (97%)	190 (97%)	6 (3%)	47 78
6	F	204/224 (91%)	200 (98%)	4 (2%)	63 86
6	S	204/224 (91%)	197 (97%)	7 (3%)	44 77

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
7	G	199/212 (94%)	192 (96%)	7 (4%)	43 76
7	T	199/212 (94%)	198 (100%)	1 (0%)	92 96
8	1	178/199 (89%)	169 (95%)	9 (5%)	29 68
8	U	178/199 (89%)	170 (96%)	8 (4%)	34 71
9	2	170/171 (99%)	168 (99%)	2 (1%)	78 90
9	V	170/171 (99%)	167 (98%)	3 (2%)	66 87
10	3	173/174 (99%)	165 (95%)	8 (5%)	33 70
10	W	173/174 (99%)	171 (99%)	2 (1%)	78 90
11	4	179/215 (83%)	172 (96%)	7 (4%)	39 74
11	X	179/215 (83%)	174 (97%)	5 (3%)	51 79
12	5	156/202 (77%)	149 (96%)	7 (4%)	34 71
12	Y	156/202 (77%)	152 (97%)	4 (3%)	54 81
13	6	155/181 (86%)	151 (97%)	4 (3%)	54 81
13	Z	155/181 (86%)	147 (95%)	8 (5%)	29 68
14	7	181/228 (79%)	178 (98%)	3 (2%)	68 88
14	8	181/228 (79%)	173 (96%)	8 (4%)	35 71
15	H	341/372 (92%)	329 (96%)	12 (4%)	43 76
16	I	336/385 (87%)	325 (97%)	11 (3%)	45 78
17	K	344/366 (94%)	336 (98%)	8 (2%)	58 83
18	L	341/341 (100%)	337 (99%)	4 (1%)	78 90
19	M	357/379 (94%)	350 (98%)	7 (2%)	63 86
20	J	339/352 (96%)	322 (95%)	17 (5%)	30 68
All	All	7270/7879 (92%)	7049 (97%)	221 (3%)	52 78

5 of 221 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	D	38	ARG
8	1	34	SER
20	J	9	MET
4	D	139	ASP
6	F	62	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
17	K	257	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 11 ligands modelled in this entry, 5 are monoatomic - leaving 6 for Mogul analysis.

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	$\#\|Z\| > 2$
21	ATP	H	501	22	26,33,33	0.83	1 (3%)	26,52,52	2.29	4 (15%)
21	ATP	I	501	22	26,33,33	0.90	1 (3%)	26,52,52	2.14	4 (15%)
23	ADP	J	501	-	24,29,29	1.02	2 (8%)	23,45,45	1.79	1 (4%)
21	ATP	K	501	22	26,33,33	1.11	1 (3%)	26,52,52	1.89	7 (26%)
21	ATP	L	401	22	26,33,33	0.98	1 (3%)	26,52,52	2.13	4 (15%)
21	ATP	M	501	22	26,33,33	1.00	0	26,52,52	2.03	3 (11%)

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
21	ATP	H	501	22	-	0/18/38/38	0/3/3/3
21	ATP	I	501	22	-	0/18/38/38	0/3/3/3
23	ADP	J	501	-	-	0/12/32/32	0/3/3/3
21	ATP	K	501	22	-	0/18/38/38	0/3/3/3
21	ATP	L	401	22	-	0/18/38/38	0/3/3/3
21	ATP	M	501	22	-	0/18/38/38	0/3/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	H	501	ATP	C5-C4	2.11	1.45	1.40
23	J	501	ADP	O4'-C1'	2.32	1.44	1.41
21	I	501	ATP	C5-C4	2.47	1.46	1.40
21	L	401	ATP	C5-C4	2.79	1.46	1.40
21	K	501	ATP	C5-C4	2.86	1.46	1.40

The worst 5 of 23 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	H	501	ATP	N3-C2-N1	-10.19	120.86	128.87
21	I	501	ATP	N3-C2-N1	-9.35	121.53	128.87
21	L	401	ATP	N3-C2-N1	-9.32	121.55	128.87
21	M	501	ATP	N3-C2-N1	-7.68	122.84	128.87
23	J	501	ADP	N3-C2-N1	-7.00	123.37	128.87

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	H	501	ATP	2	0
23	J	501	ADP	2	0
21	K	501	ATP	5	0
21	L	401	ATP	1	0
21	M	501	ATP	4	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.