wwPDB X-ray Structure Validation Summary Report (i)

Apr 21, 2025 – 11:01 AM EDT

PDB ID	:	9C97 / pdb_00009c97
Title	:	Yeast 20S proteasome soaked with BRA-346 fraction
Authors	:	Meneghello, R.; Rustiguel, J.K.
Deposited on	:	2024-06-13
Resolution	:	3.33 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 (i) 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 (1)) were used in the production of this report:

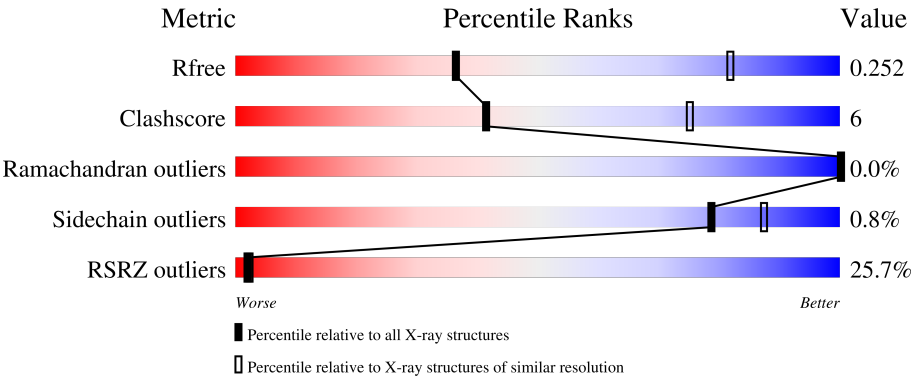
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.42

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.33 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}	164625	1325 (3.38-3.30)
Clashscore	180529	1376 (3.38-3.30)
Ramachandran outliers	177936	1376 (3.38-3.30)
Sidechain outliers	177891	1375 (3.38-3.30)
RSRZ outliers	164620	1325 (3.38-3.30)

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 <=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	30% 85% 14%
1	O	250	26% 80% 20%
2	B	258	35% 79% 15% 6%
2	P	258	28% 78% 16% 5%
3	C	254	43% 74% 19% 7%

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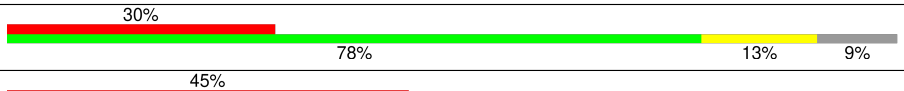
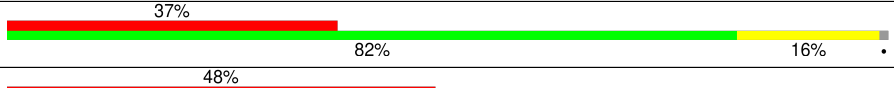
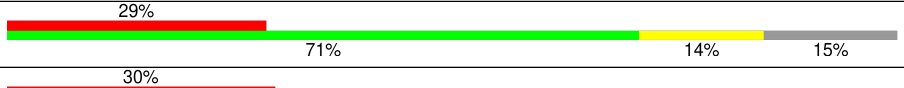
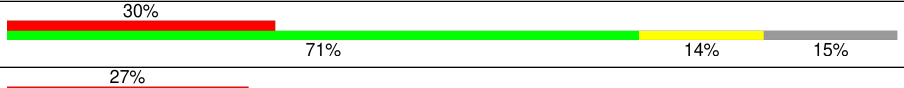
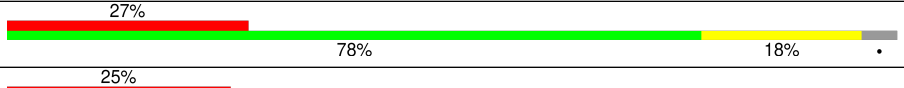
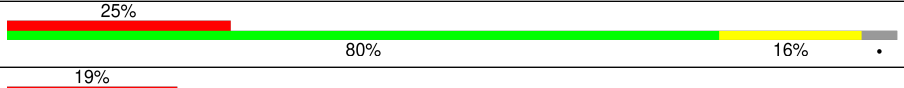
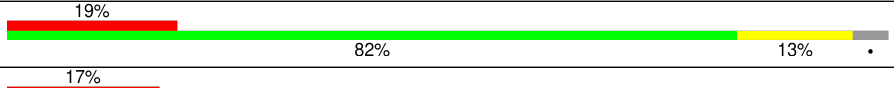
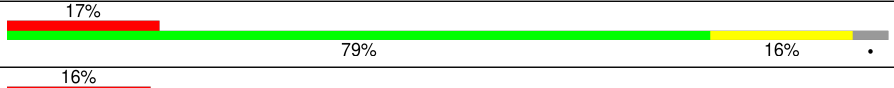
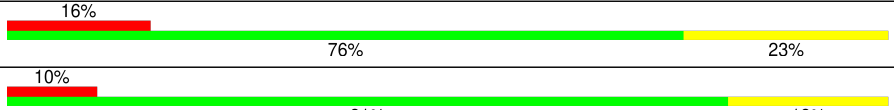
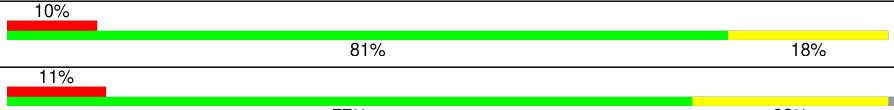
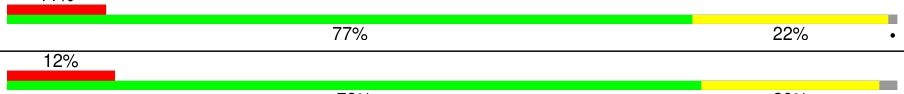
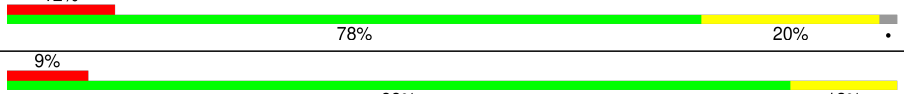
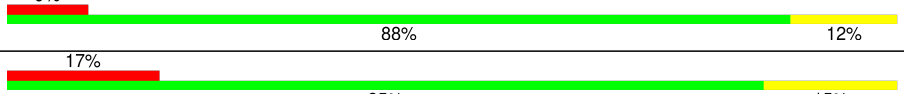
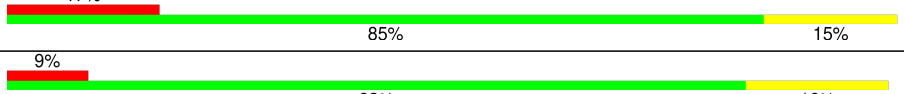
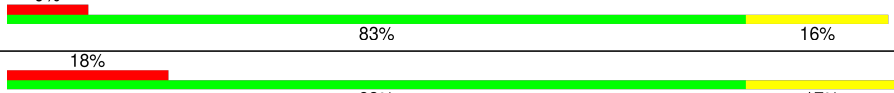
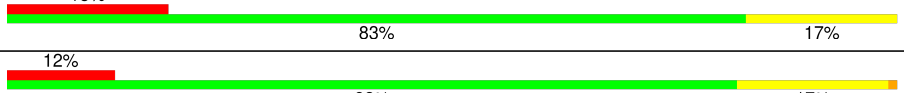
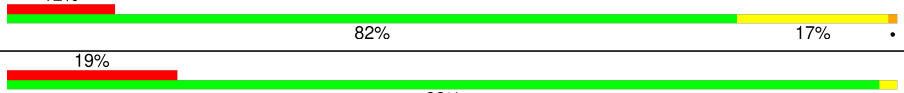
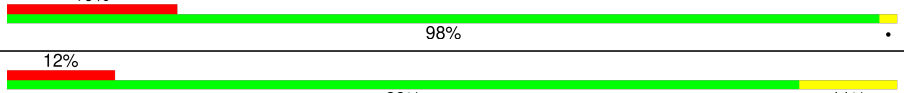
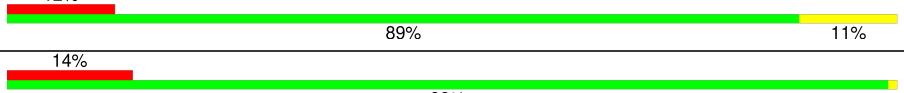
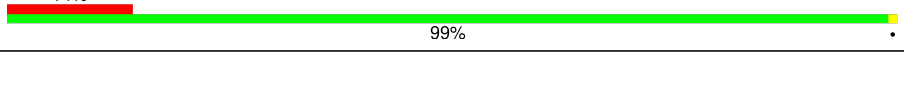
Mol	Chain	Length	Quality of chain
3	Q	254	
4	D	260	
4	R	260	
5	E	234	
5	S	234	
6	F	287	
6	T	287	
7	G	252	
7	U	252	
8	H	232	
8	V	232	
9	I	205	
9	W	205	
10	J	198	
10	X	198	
11	K	212	
11	Y	212	
12	L	222	
12	Z	222	
13	M	233	
13	a	233	
14	N	196	
14	b	196	

2 Entry composition (i)

There are 17 unique types of molecules in this entry. The entry contains 49866 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 PRE8 isoform 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	249	Total	C	N	O	S	0	0	0
			1907	1214	314	376	3			
1	O	249	Total	C	N	O	S	0	0	0
			1907	1214	314	376	3			

- Molecule 2 is a protein called PRE9 isoform 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	242	Total	C	N	O	S	0	0	0
			1894	1197	319	375	3			
2	P	244	Total	C	N	O	S	0	0	0
			1909	1206	322	378	3			

- Molecule 3 is a protein called PRE6 isoform 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	236	Total	C	N	O	S	0	0	0
			1848	1156	324	364	4			
3	Q	239	Total	C	N	O	S	0	0	0
			1875	1171	329	371	4			

- Molecule 4 is a protein called PUP2 isoform 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	237	Total	C	N	O	S	0	0	0
			1836	1151	309	369	7			
4	R	239	Total	C	N	O	S	0	0	0
			1850	1159	311	373	7			

- Molecule 5 is a protein called PRE5 isoform 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	231	Total	C	N	O	S	0	0	0
			1770	1113	307	346	4			
5	S	232	Total	C	N	O	S	0	0	0
			1784	1120	311	349	4			

- Molecule 6 is a protein called PRE10 isoform 1.

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
			1894	1204	330	356	4			

- Molecule 7 is a protein called SCL1 isoform 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	241	Total	C	N	O	S	0	0	0
			1907	1214	320	365	8			
7	U	242	Total	C	N	O	S	0	0	0
			1913	1217	321	367	8			

- Molecule 8 is a protein called proteasome endopeptidase complex.

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
			1680	1060	293	321	6			

- Molecule 9 is a protein called PUP3 isoform 1.

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

- Molecule 10 is a protein called Proteasome subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	196	Total	C	N	O	S	0	0	0
			1570	997	266	301	6			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	X	195	Total	C	N	O	S	0	0	0
			1561	992	264	299	6			

- Molecule 11 is a protein called proteasome endopeptidase complex.

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 PRE7 isoform 1.

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

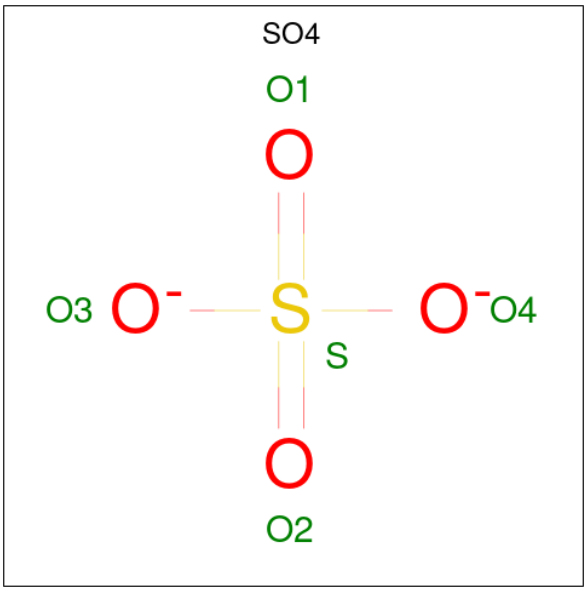
- Molecule 13 is a protein called Proteasome subunit beta.

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

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

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

- Molecule 15 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	B	1	Total O S 5 4 1	0	0
15	C	1	Total O S 5 4 1	0	0
15	D	1	Total O S 5 4 1	0	0
15	E	1	Total O S 5 4 1	0	0
15	E	1	Total O S 5 4 1	0	0
15	E	1	Total O S 5 4 1	0	0
15	E	1	Total O S 5 4 1	0	0
15	F	1	Total O S 5 4 1	0	0
15	F	1	Total O S 5 4 1	0	0
15	G	1	Total O S 5 4 1	0	0
15	G	1	Total O S 5 4 1	0	0
15	P	1	Total O S 5 4 1	0	0
15	P	1	Total O S 5 4 1	0	0
15	Q	1	Total O S 5 4 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	R	1	Total O S 5 4 1	0	0
15	S	1	Total O S 5 4 1	0	0
15	S	1	Total O S 5 4 1	0	0
15	T	1	Total O S 5 4 1	0	0
15	U	1	Total O S 5 4 1	0	0
15	H	1	Total O S 5 4 1	0	0
15	H	1	Total O S 5 4 1	0	0
15	I	1	Total O S 5 4 1	0	0
15	J	1	Total O S 5 4 1	0	0
15	J	1	Total O S 5 4 1	0	0
15	K	1	Total O S 5 4 1	0	0
15	K	1	Total O S 5 4 1	0	0
15	K	1	Total O S 5 4 1	0	0
15	L	1	Total O S 5 4 1	0	0
15	L	1	Total O S 5 4 1	0	0
15	M	1	Total O S 5 4 1	0	0
15	M	1	Total O S 5 4 1	0	0
15	M	1	Total O S 5 4 1	0	0
15	M	1	Total O S 5 4 1	0	0
15	N	1	Total O S 5 4 1	0	0
15	N	1	Total O S 5 4 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	V	1	Total O S 5 4 1	0	0
15	X	1	Total O S 5 4 1	0	0
15	Z	1	Total O S 5 4 1	0	0
15	Z	1	Total O S 5 4 1	0	0
15	a	1	Total O S 5 4 1	0	0
15	a	1	Total O S 5 4 1	0	0
15	a	1	Total O S 5 4 1	0	0
15	a	1	Total O S 5 4 1	0	0
15	b	1	Total O S 5 4 1	0	0

- Molecule 16 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	H	1	Total Mg 1 1	0	0
16	I	1	Total Mg 1 1	0	0
16	K	1	Total Mg 1 1	0	0
16	L	1	Total Mg 1 1	0	0
16	N	1	Total Mg 1 1	0	0
16	V	1	Total Mg 1 1	0	0
16	W	1	Total Mg 1 1	0	0
16	Y	1	Total Mg 1 1	0	0
16	Z	1	Total Mg 1 1	0	0

- Molecule 17 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	A	7	Total O 7 7	0	0
17	B	12	Total O 12 12	0	0
17	C	5	Total O 5 5	0	0
17	D	11	Total O 11 11	0	0
17	E	5	Total O 5 5	0	0
17	F	11	Total O 11 11	0	0
17	G	14	Total O 14 14	0	0
17	O	9	Total O 9 9	0	0
17	P	9	Total O 9 9	0	0
17	Q	2	Total O 2 2	0	0
17	R	9	Total O 9 9	0	0
17	S	12	Total O 12 12	0	0
17	T	10	Total O 10 10	0	0
17	U	11	Total O 11 11	0	0
17	H	19	Total O 19 19	0	0
17	I	8	Total O 8 8	0	0
17	J	19	Total O 19 19	0	0
17	K	7	Total O 7 7	0	0
17	L	11	Total O 11 11	0	0
17	M	11	Total O 11 11	0	0
17	N	7	Total O 7 7	0	0
17	V	8	Total O 8 8	0	0

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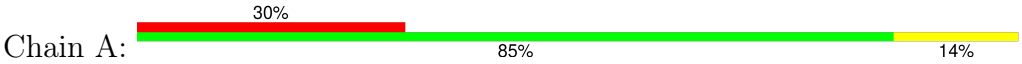
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	W	16	Total O 16 16	0	0
17	X	13	Total O 13 13	0	0
17	Y	7	Total O 7 7	0	0
17	Z	21	Total O 21 21	0	0
17	a	27	Total O 27 27	0	0
17	b	15	Total O 15 15	0	0

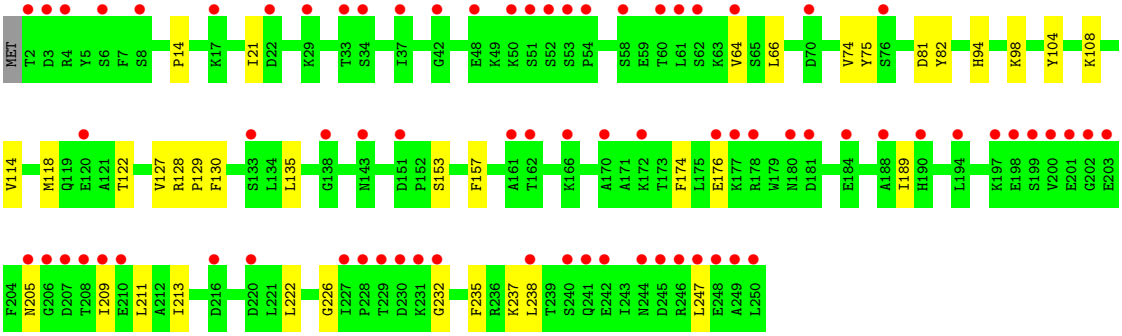
3 Residue-property plots (i)

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: PRE8 isoform 1

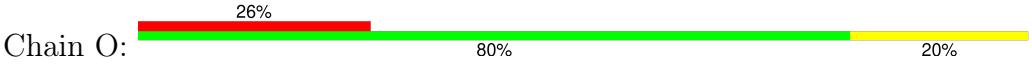
Chain A:

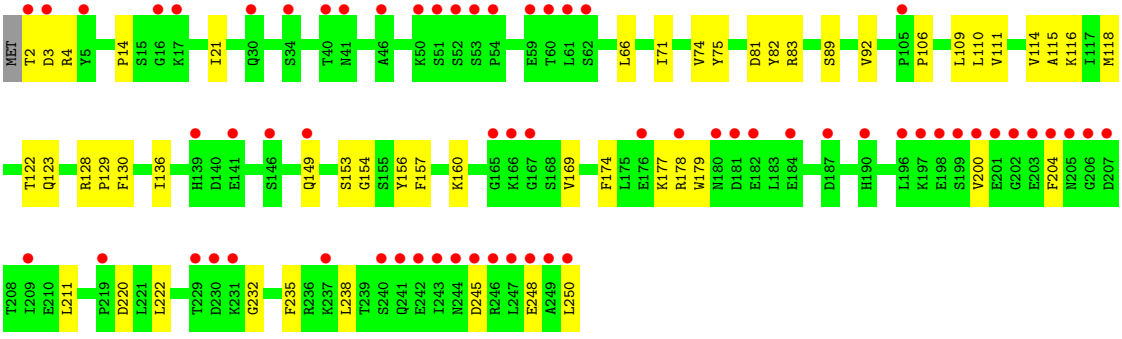




• Molecule 1: PRE8 isoform 1

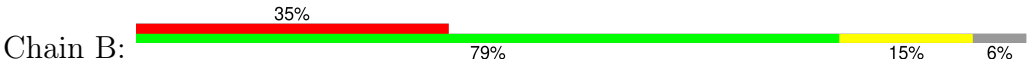
Chain O:

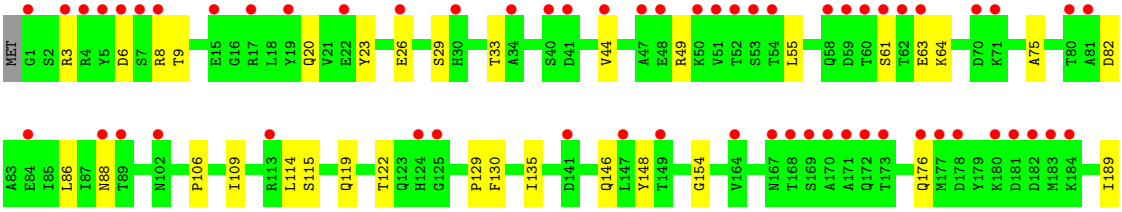


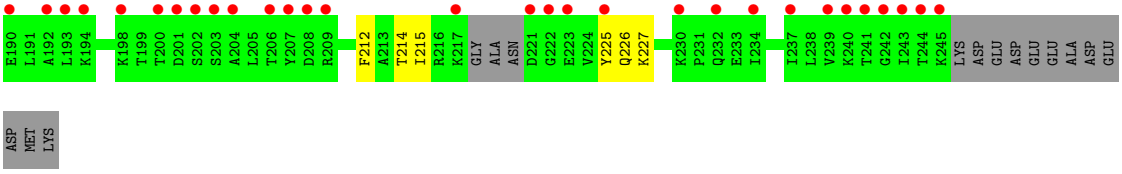


• Molecule 2: PRE9 isoform 1

Chain B:

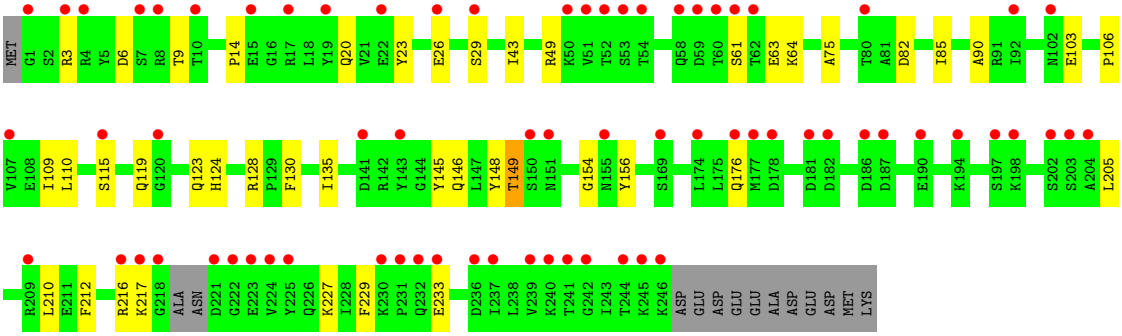






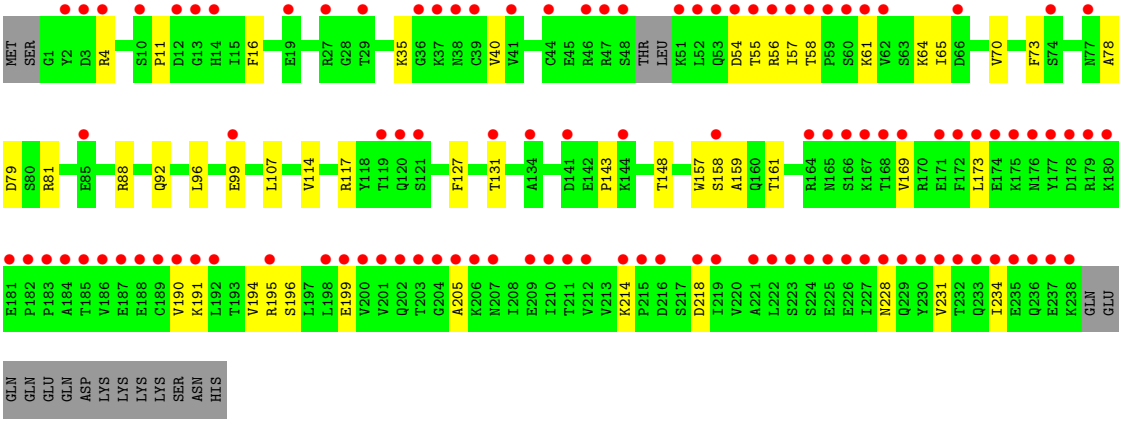
• Molecule 2: PRE9 isoform 1

Chain P:



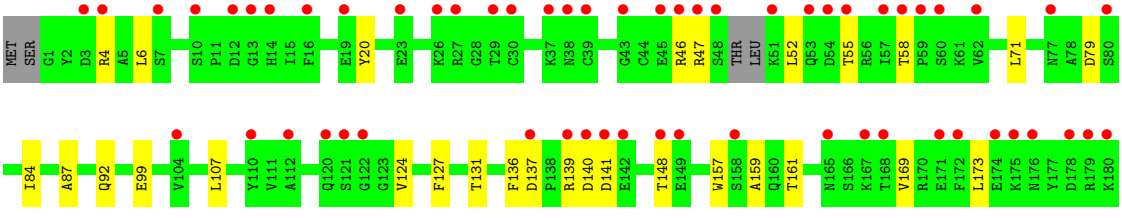
• Molecule 3: PRE6 isoform 1

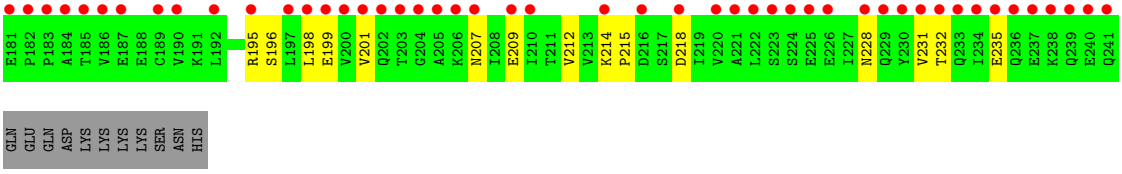
Chain C:



• Molecule 3: PRE6 isoform 1

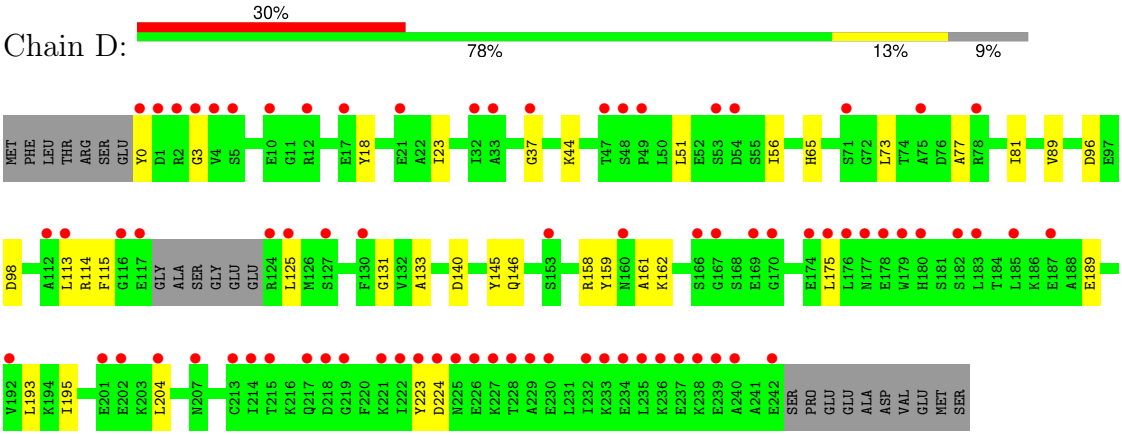
Chain Q:





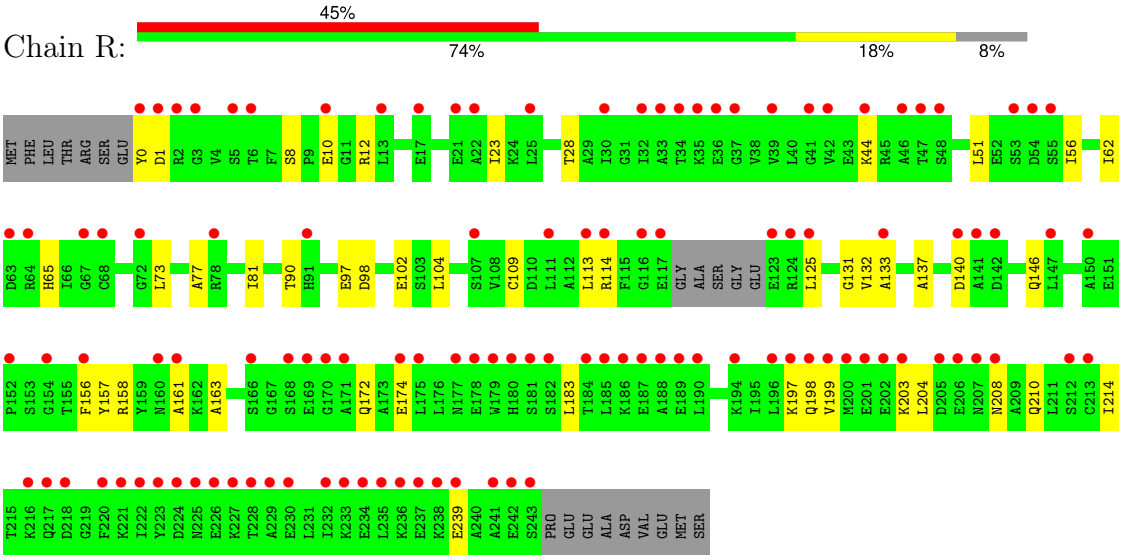
• Molecule 4: PUP2 isoform 1

Chain D:



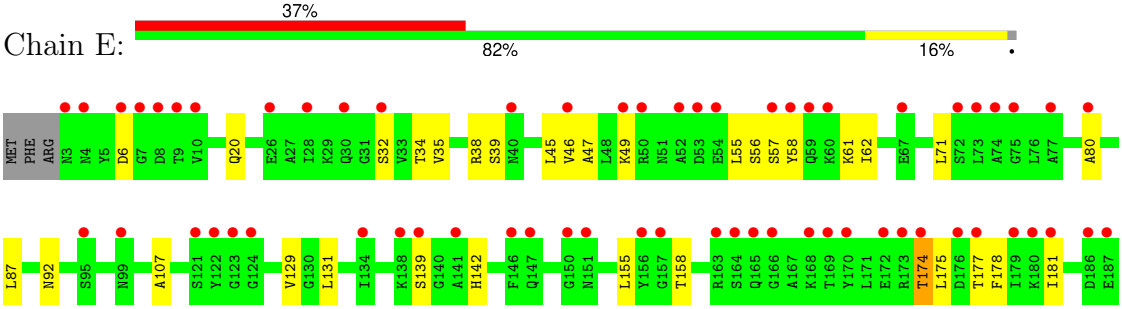
• Molecule 4: PUP2 isoform 1

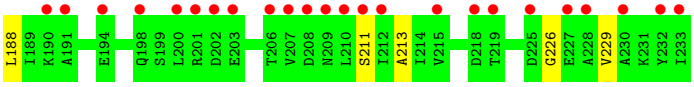
Chain R:



• Molecule 5: PRE5 isoform 1

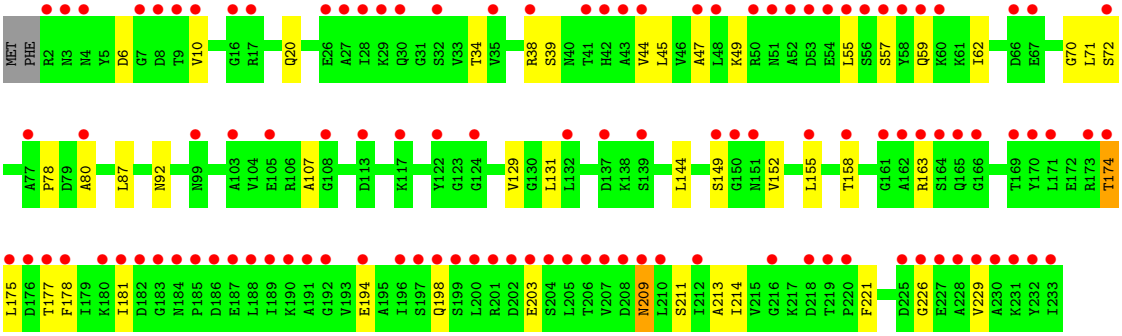
Chain E:





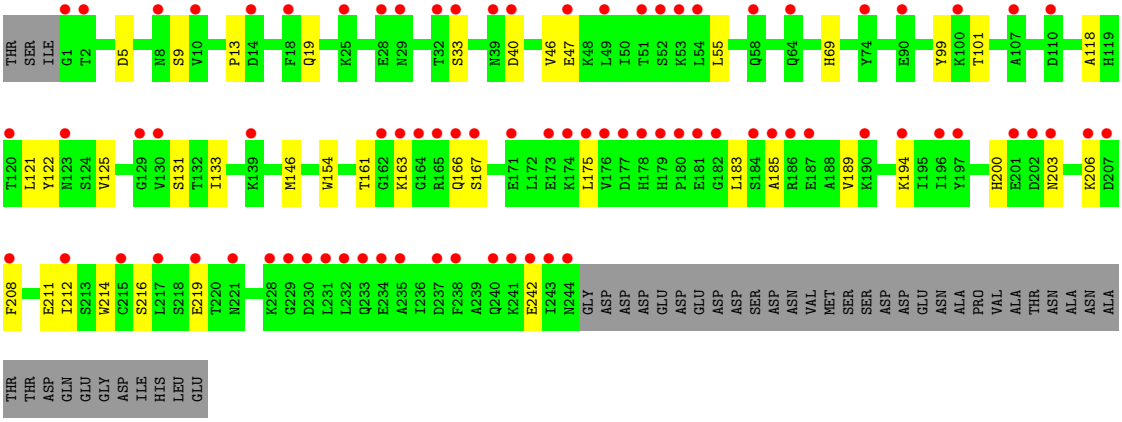
• Molecule 5: PRE5 isoform 1

Chain S:



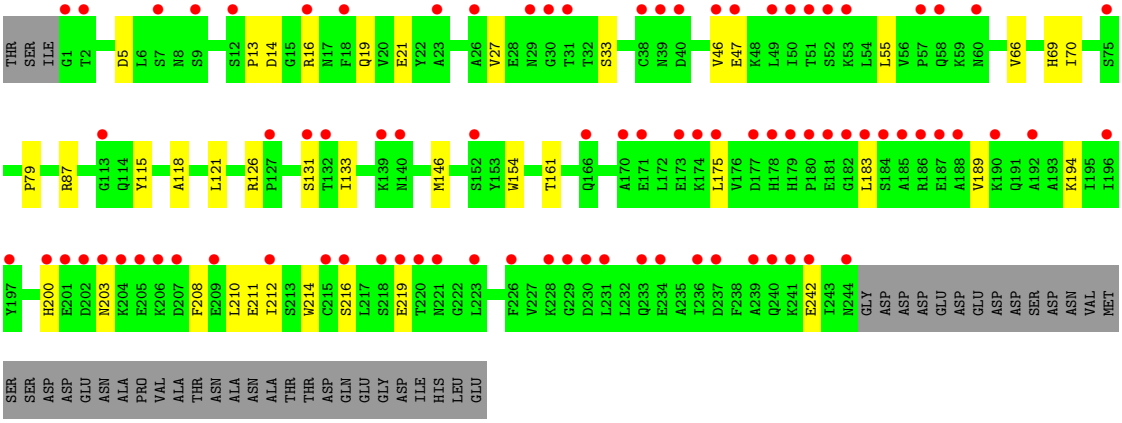
• Molecule 6: PRE10 isoform 1

Chain F:



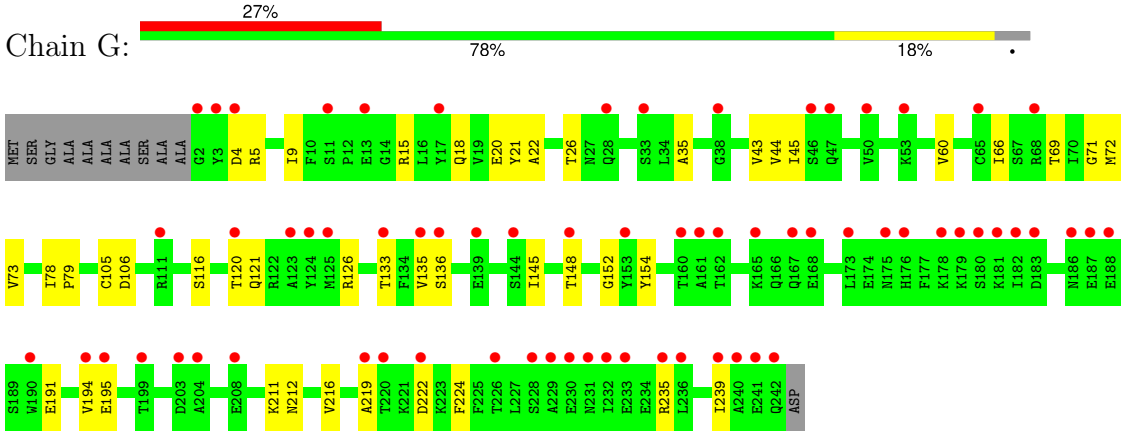
• Molecule 6: PRE10 isoform 1

Chain T:



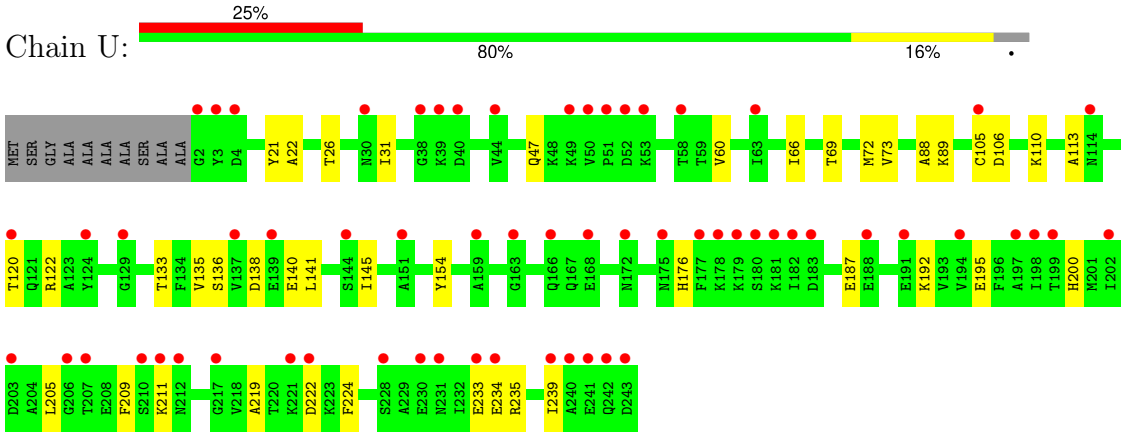
• Molecule 7: SCL1 isoform 1

Chain G:



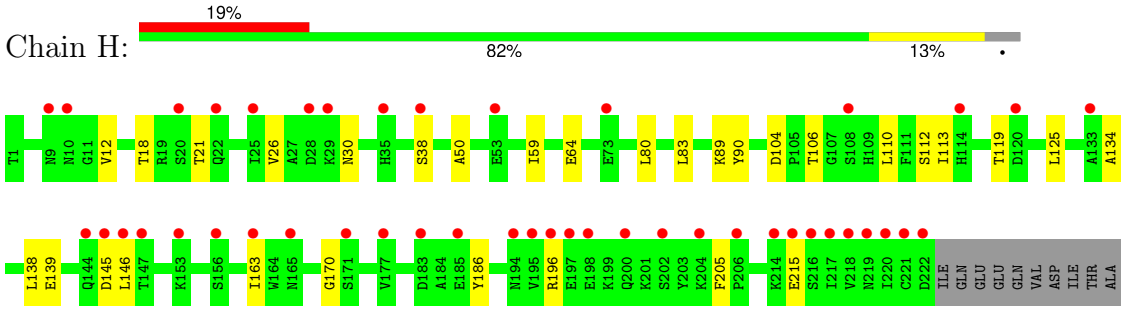
• Molecule 7: SCL1 isoform 1

Chain U:



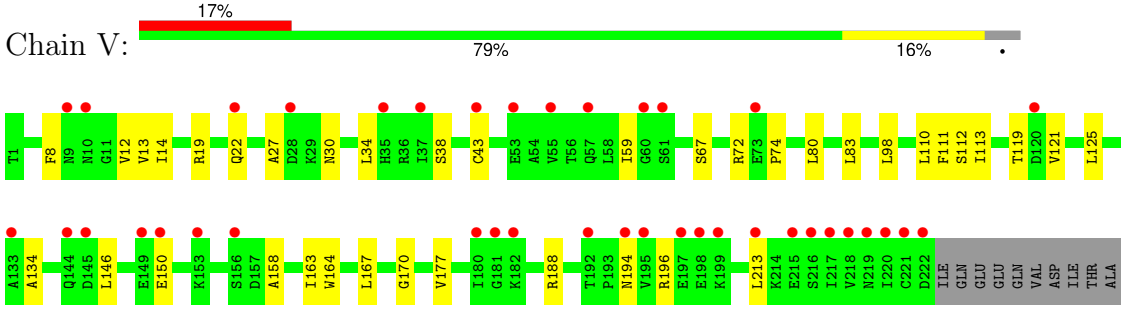
• Molecule 8: proteasome endopeptidase complex

Chain H:



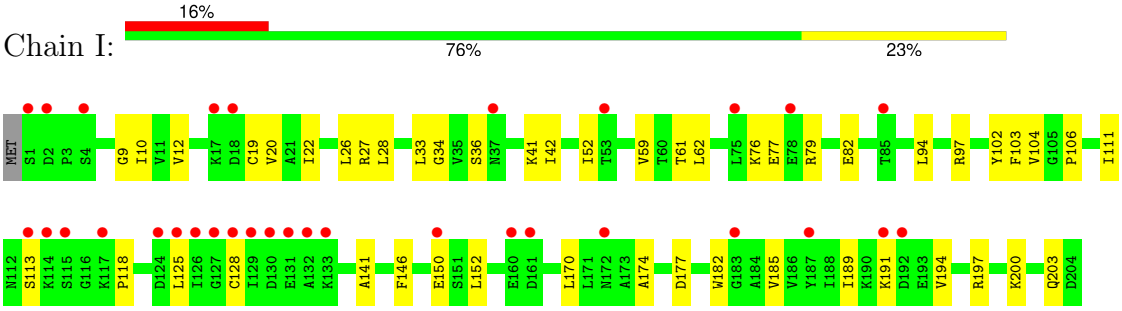
• Molecule 8: proteasome endopeptidase complex

Chain V:



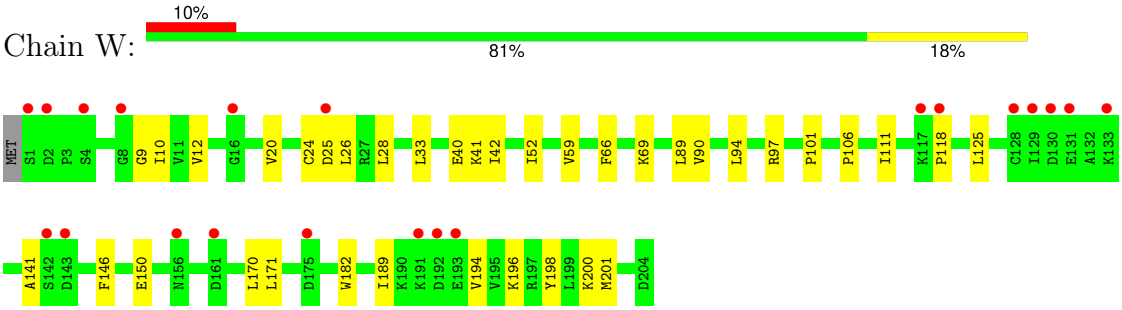
• Molecule 9: PUP3 isoform 1

Chain I:



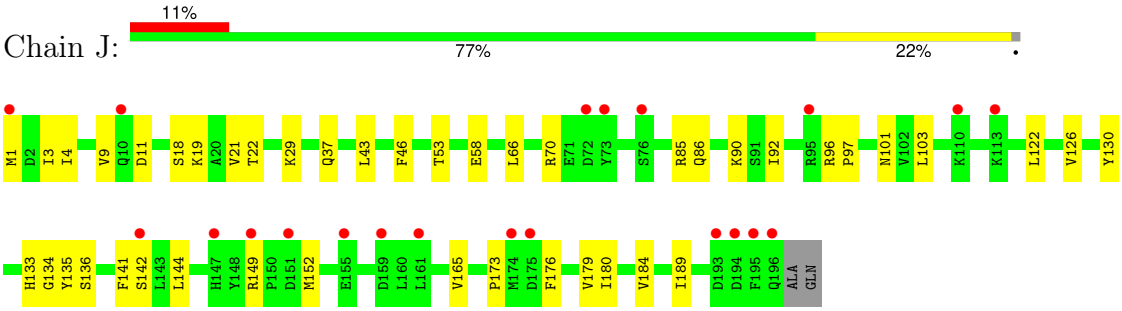
• Molecule 9: PUP3 isoform 1

Chain W:



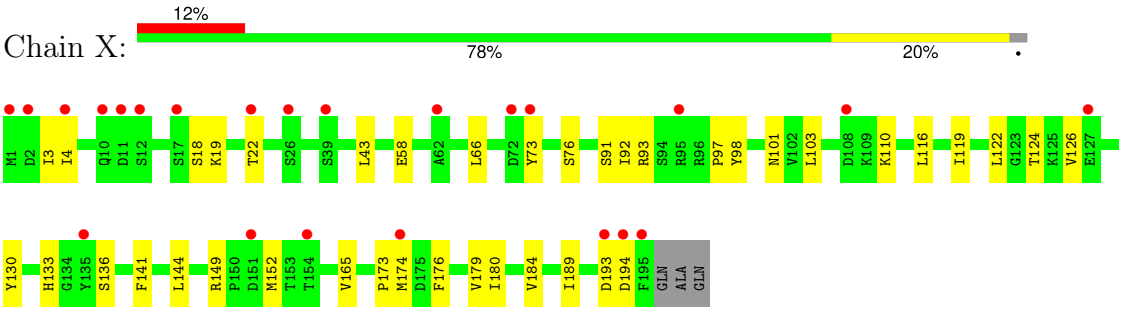
• Molecule 10: Proteasome subunit beta

Chain J:



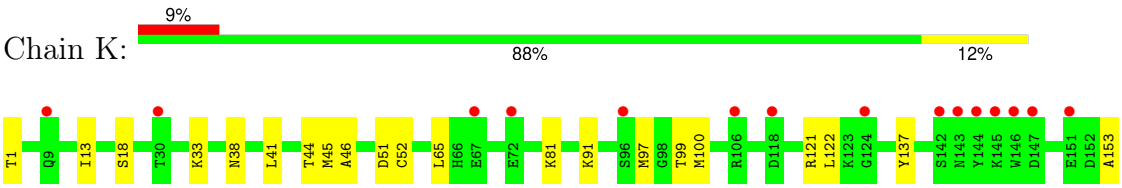
• Molecule 10: Proteasome subunit beta

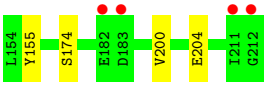
Chain X:



• Molecule 11: proteasome endopeptidase complex

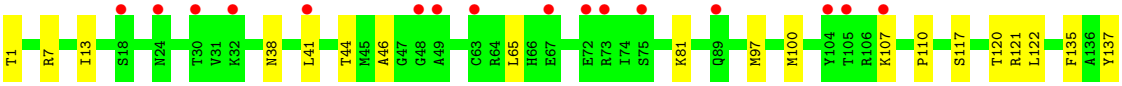
Chain K:





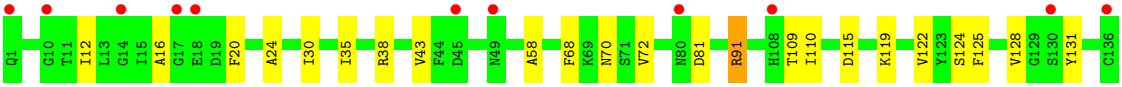
• Molecule 11: proteasome endopeptidase complex

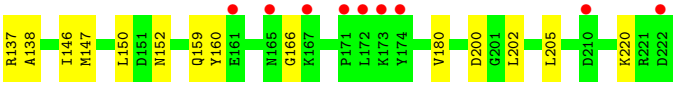
Chain Y:



• Molecule 12: PRE7 isoform 1

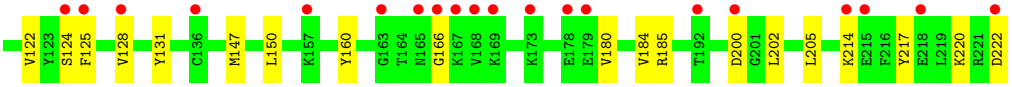
Chain L:





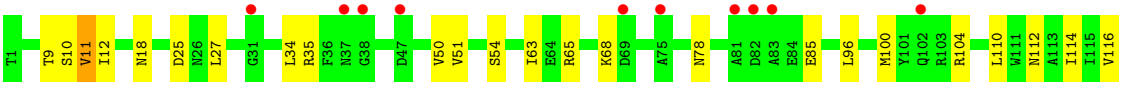
• Molecule 12: PRE7 isoform 1

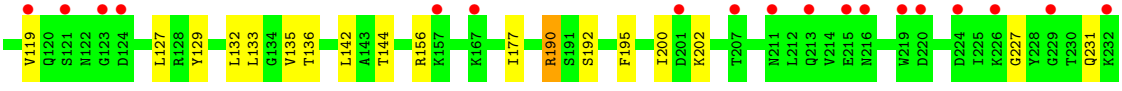
Chain Z:



• Molecule 13: Proteasome subunit beta

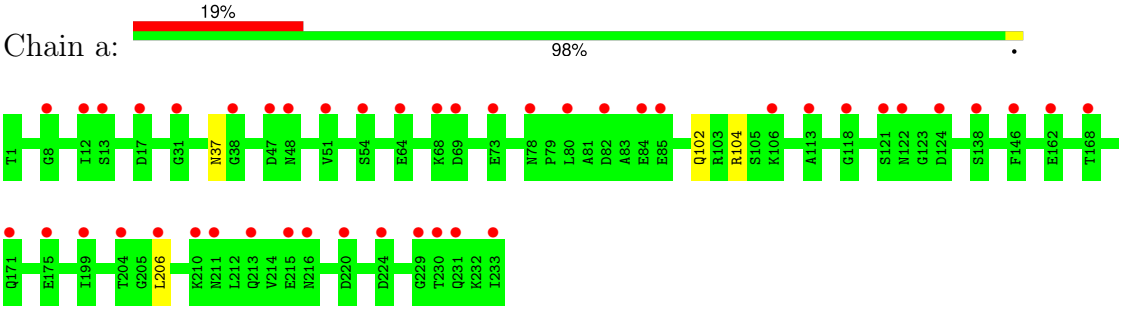
Chain M:





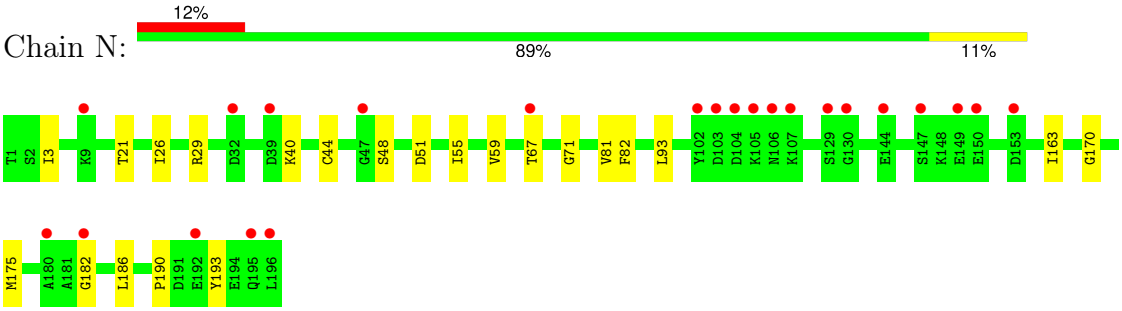
• Molecule 13: Proteasome subunit beta

Chain a:



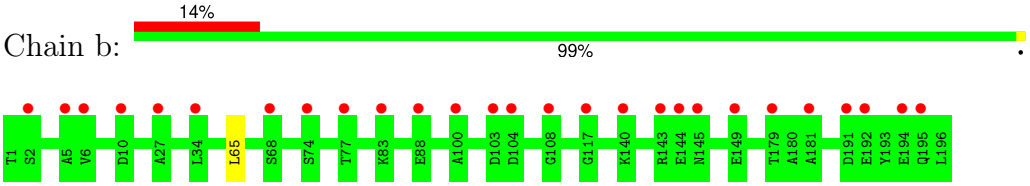
• Molecule 14: Proteasome subunit beta type-1

Chain N:



• Molecule 14: Proteasome subunit beta type-1

Chain b:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	117.51Å 299.92Å 143.91Å 90.00° 108.46° 90.00°	Depositor
Resolution (Å)	49.11 – 3.33 49.11 – 3.33	Depositor EDS
% Data completeness (in resolution range)	96.0 (49.11-3.33) 86.4 (49.11-3.33)	Depositor EDS
R_{merge}	0.40	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.08 (at 3.33Å)	Xtriage
Refinement program	PHENIX 1.21_5207	Depositor
R, R_{free}	0.200 , 0.252 0.201 , 0.252	Depositor DCC
R_{free} test set	6918 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	-19.1	Xtriage
Anisotropy	-2.049	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 52.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.87	EDS
Total number of atoms	49866	wwPDB-VP
Average B, all atoms (Å^2)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.27% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, SO4

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	0.25	0/1944	0.47	0/2632
1	O	0.25	0/1944	0.47	0/2632
2	B	0.24	0/1923	0.48	0/2600
2	P	0.24	0/1938	0.49	0/2619
3	C	0.24	0/1876	0.49	0/2538
3	Q	0.24	0/1903	0.49	0/2574
4	D	0.24	0/1861	0.48	0/2507
4	R	0.24	0/1875	0.46	0/2526
5	E	0.24	0/1797	0.48	0/2429
5	S	0.24	0/1811	0.49	0/2447
6	F	0.25	0/1936	0.46	0/2614
6	T	0.25	0/1934	0.46	0/2611
7	G	0.25	0/1945	0.46	0/2634
7	U	0.26	0/1951	0.46	0/2641
8	H	0.24	0/1715	0.46	0/2326
8	V	0.25	0/1711	0.46	0/2321
9	I	0.25	0/1611	0.49	0/2174
9	W	0.25	0/1611	0.49	0/2174
10	J	0.25	0/1598	0.48	0/2154
10	X	0.25	0/1589	0.48	0/2142
11	K	0.25	0/1681	0.48	0/2274
11	Y	0.25	0/1681	0.47	0/2274
12	L	0.26	0/1795	0.49	0/2420
12	Z	0.25	0/1795	0.48	0/2420
13	M	0.25	0/1855	0.51	0/2514
13	a	0.25	0/1855	0.49	0/2514
14	N	0.24	0/1541	0.46	0/2087
14	b	0.25	0/1541	0.48	0/2087
All	All	0.25	0/50217	0.48	0/67885

There are no bond length outliers.

There are no bond angle outliers.

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	1907	0	1917	23	0
1	O	1907	0	1917	30	0
2	B	1894	0	1897	26	0
2	P	1909	0	1918	27	0
3	C	1848	0	1862	35	0
3	Q	1875	0	1884	28	0
4	D	1836	0	1819	27	0
4	R	1850	0	1827	32	0
5	E	1770	0	1773	25	0
5	S	1784	0	1788	29	0
6	F	1896	0	1889	23	0
6	T	1894	0	1884	23	0
7	G	1907	0	1901	27	0
7	U	1913	0	1903	29	0
8	H	1684	0	1688	19	0
8	V	1680	0	1683	27	0
9	I	1581	0	1574	34	0
9	W	1581	0	1574	24	0
10	J	1570	0	1577	34	0
10	X	1561	0	1569	27	0
11	K	1644	0	1595	17	0
11	Y	1644	0	1595	20	0
12	L	1757	0	1711	23	0
12	Z	1757	0	1710	22	0
13	M	1824	0	1832	27	0
13	a	1824	0	1832	0	0
14	N	1512	0	1481	12	0
14	b	1512	0	1481	0	0
15	B	5	0	0	0	0
15	C	5	0	0	0	0
15	D	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	E	20	0	0	0	0
15	F	10	0	0	0	0
15	G	10	0	0	0	0
15	H	10	0	0	0	0
15	I	5	0	0	0	0
15	J	10	0	0	0	0
15	K	15	0	0	0	0
15	L	10	0	0	0	0
15	M	20	0	0	0	0
15	N	10	0	0	1	0
15	P	10	0	0	0	0
15	Q	5	0	0	0	0
15	R	5	0	0	1	0
15	S	10	0	0	0	0
15	T	5	0	0	0	0
15	U	5	0	0	0	0
15	V	5	0	0	0	0
15	X	5	0	0	0	0
15	Z	10	0	0	0	0
15	a	20	0	0	0	0
15	b	5	0	0	0	0
16	H	1	0	0	0	0
16	I	1	0	0	0	0
16	K	1	0	0	0	0
16	L	1	0	0	0	0
16	N	1	0	0	0	0
16	V	1	0	0	0	0
16	W	1	0	0	0	0
16	Y	1	0	0	0	0
16	Z	1	0	0	0	0
17	A	7	0	0	1	0
17	B	12	0	0	1	0
17	C	5	0	0	0	0
17	D	11	0	0	0	0
17	E	5	0	0	0	0
17	F	11	0	0	0	0
17	G	14	0	0	0	0
17	H	19	0	0	0	0
17	I	8	0	0	0	0
17	J	19	0	0	0	0
17	K	7	0	0	0	0
17	L	11	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	M	11	0	0	1	0
17	N	7	0	0	0	0
17	O	9	0	0	0	0
17	P	9	0	0	0	0
17	Q	2	0	0	0	0
17	R	9	0	0	0	0
17	S	12	0	0	0	0
17	T	10	0	0	0	0
17	U	11	0	0	0	0
17	V	8	0	0	0	0
17	W	16	0	0	0	0
17	X	13	0	0	0	0
17	Y	7	0	0	0	0
17	Z	21	0	0	0	0
17	a	27	0	0	0	0
17	b	15	0	0	0	0
All	All	49866	0	49081	573	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 573 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)
5:S:80:ALA:HB2	5:S:129:VAL:HG21	1.66	0.75
5:E:80:ALA:HB2	5:E:129:VAL:HG21	1.69	0.75
10:J:173:PRO:HB3	10:X:22:THR:HG21	1.69	0.75
3:C:79:ASP:HB3	3:C:127:PHE:HD1	1.55	0.71
4:D:96:ASP:HB2	12:L:91:ARG:HG3	1.72	0.71

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	247/250 (99%)	235 (95%)	12 (5%)	0	100	100
1	O	247/250 (99%)	237 (96%)	10 (4%)	0	100	100
2	B	238/258 (92%)	232 (98%)	6 (2%)	0	100	100
2	P	240/258 (93%)	235 (98%)	5 (2%)	0	100	100
3	C	232/254 (91%)	226 (97%)	6 (3%)	0	100	100
3	Q	235/254 (92%)	227 (97%)	8 (3%)	0	100	100
4	D	233/260 (90%)	227 (97%)	6 (3%)	0	100	100
4	R	235/260 (90%)	229 (97%)	6 (3%)	0	100	100
5	E	229/234 (98%)	222 (97%)	7 (3%)	0	100	100
5	S	230/234 (98%)	225 (98%)	5 (2%)	0	100	100
6	F	242/287 (84%)	234 (97%)	8 (3%)	0	100	100
6	T	242/287 (84%)	232 (96%)	10 (4%)	0	100	100
7	G	239/252 (95%)	229 (96%)	10 (4%)	0	100	100
7	U	240/252 (95%)	230 (96%)	10 (4%)	0	100	100
8	H	220/232 (95%)	209 (95%)	9 (4%)	2 (1%)	14	44
8	V	220/232 (95%)	212 (96%)	8 (4%)	0	100	100
9	I	202/205 (98%)	191 (95%)	11 (5%)	0	100	100
9	W	202/205 (98%)	192 (95%)	10 (5%)	0	100	100
10	J	194/198 (98%)	186 (96%)	8 (4%)	0	100	100
10	X	193/198 (98%)	185 (96%)	8 (4%)	0	100	100
11	K	210/212 (99%)	205 (98%)	5 (2%)	0	100	100
11	Y	210/212 (99%)	205 (98%)	5 (2%)	0	100	100
12	L	220/222 (99%)	213 (97%)	7 (3%)	0	100	100
12	Z	220/222 (99%)	214 (97%)	6 (3%)	0	100	100
13	M	231/233 (99%)	221 (96%)	10 (4%)	0	100	100
13	a	231/233 (99%)	221 (96%)	10 (4%)	0	100	100
14	N	194/196 (99%)	187 (96%)	7 (4%)	0	100	100
14	b	194/196 (99%)	189 (97%)	5 (3%)	0	100	100
All	All	6270/6586 (95%)	6050 (96%)	218 (4%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	H	145	ASP
8	H	146	LEU

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	208/209 (100%)	206 (99%)	2 (1%)	73	84
1	O	208/209 (100%)	206 (99%)	2 (1%)	73	84
2	B	202/216 (94%)	201 (100%)	1 (0%)	86	91
2	P	204/216 (94%)	203 (100%)	1 (0%)	86	91
3	C	208/226 (92%)	208 (100%)	0	100	100
3	Q	211/226 (93%)	208 (99%)	3 (1%)	62	78
4	D	196/215 (91%)	196 (100%)	0	100	100
4	R	197/215 (92%)	196 (100%)	1 (0%)	86	91
5	E	189/193 (98%)	187 (99%)	2 (1%)	70	82
5	S	191/193 (99%)	188 (98%)	3 (2%)	58	75
6	F	201/238 (84%)	199 (99%)	2 (1%)	73	84
6	T	200/238 (84%)	197 (98%)	3 (2%)	60	77
7	G	206/210 (98%)	206 (100%)	0	100	100
7	U	206/210 (98%)	206 (100%)	0	100	100
8	H	181/190 (95%)	180 (99%)	1 (1%)	84	90
8	V	179/190 (94%)	178 (99%)	1 (1%)	84	90
9	I	172/173 (99%)	171 (99%)	1 (1%)	84	90
9	W	172/173 (99%)	170 (99%)	2 (1%)	67	80
10	J	174/175 (99%)	173 (99%)	1 (1%)	84	90
10	X	173/175 (99%)	172 (99%)	1 (1%)	84	90
11	K	169/169 (100%)	168 (99%)	1 (1%)	84	90
11	Y	169/169 (100%)	167 (99%)	2 (1%)	67	80

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
12	L	185/185 (100%)	182 (98%)	3 (2%)	58 75
12	Z	185/185 (100%)	184 (100%)	1 (0%)	86 91
13	M	199/199 (100%)	196 (98%)	3 (2%)	60 77
13	a	199/199 (100%)	195 (98%)	4 (2%)	50 72
14	N	162/162 (100%)	162 (100%)	0	100 100
14	b	162/162 (100%)	161 (99%)	1 (1%)	84 90
All	All	5308/5520 (96%)	5266 (99%)	42 (1%)	79 87

5 of 42 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
13	M	127	LEU
11	Y	137	TYR
13	M	190	ARG
9	W	182	TRP
13	a	37	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 53 ligands modelled in this entry, 9 are monoatomic - leaving 44 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	$\#\|Z\| > 2$
15	SO4	L	303	-	4,4,4	0.68	0	6,6,6	0.09	0
15	SO4	E	304	-	4,4,4	0.67	0	6,6,6	0.08	0
15	SO4	a	304	-	4,4,4	0.68	0	6,6,6	0.12	0
15	SO4	H	302	-	4,4,4	0.68	0	6,6,6	0.10	0
15	SO4	S	302	-	4,4,4	0.68	0	6,6,6	0.09	0
15	SO4	K	303	-	4,4,4	0.68	0	6,6,6	0.07	0
15	SO4	N	201	-	4,4,4	0.66	0	6,6,6	0.09	0
15	SO4	a	303	-	4,4,4	0.68	0	6,6,6	0.12	0
15	SO4	B	301	-	4,4,4	0.68	0	6,6,6	0.07	0
15	SO4	Z	302	-	4,4,4	0.68	0	6,6,6	0.10	0
15	SO4	M	301	-	4,4,4	0.67	0	6,6,6	0.08	0
15	SO4	M	304	-	4,4,4	0.68	0	6,6,6	0.06	0
15	SO4	Z	303	-	4,4,4	0.68	0	6,6,6	0.08	0
15	SO4	M	303	-	4,4,4	0.68	0	6,6,6	0.10	0
15	SO4	S	301	-	4,4,4	0.67	0	6,6,6	0.07	0
15	SO4	D	301	-	4,4,4	0.67	0	6,6,6	0.07	0
15	SO4	b	201	-	4,4,4	0.67	0	6,6,6	0.10	0
15	SO4	K	304	-	4,4,4	0.68	0	6,6,6	0.06	0
15	SO4	F	302	-	4,4,4	0.67	0	6,6,6	0.08	0
15	SO4	J	201	-	4,4,4	0.67	0	6,6,6	0.08	0
15	SO4	a	301	-	4,4,4	0.68	0	6,6,6	0.09	0
15	SO4	I	302	-	4,4,4	0.67	0	6,6,6	0.08	0
15	SO4	Q	301	-	4,4,4	0.67	0	6,6,6	0.11	0
15	SO4	J	202	-	4,4,4	0.67	0	6,6,6	0.10	0
15	SO4	G	301	-	4,4,4	0.68	0	6,6,6	0.11	0
15	SO4	P	302	-	4,4,4	0.67	0	6,6,6	0.06	0
15	SO4	X	201	-	4,4,4	0.67	0	6,6,6	0.11	0
15	SO4	E	302	-	4,4,4	0.68	0	6,6,6	0.10	0
15	SO4	a	302	-	4,4,4	0.67	0	6,6,6	0.08	0
15	SO4	M	302	-	4,4,4	0.68	0	6,6,6	0.08	0
15	SO4	E	301	-	4,4,4	0.67	0	6,6,6	0.06	0
15	SO4	F	301	-	4,4,4	0.67	0	6,6,6	0.08	0
15	SO4	C	301	-	4,4,4	0.67	0	6,6,6	0.09	0
15	SO4	R	301	-	4,4,4	0.68	0	6,6,6	0.07	0
15	SO4	U	301	-	4,4,4	0.68	0	6,6,6	0.12	0
15	SO4	P	301	-	4,4,4	0.67	0	6,6,6	0.09	0
15	SO4	L	302	-	4,4,4	0.68	0	6,6,6	0.09	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
15	SO4	V	302	-	4,4,4	0.68	0	6,6,6	0.09	0
15	SO4	G	302	-	4,4,4	0.68	0	6,6,6	0.09	0
15	SO4	H	303	-	4,4,4	0.67	0	6,6,6	0.06	0
15	SO4	E	303	-	4,4,4	0.67	0	6,6,6	0.09	0
15	SO4	T	301	-	4,4,4	0.67	0	6,6,6	0.10	0
15	SO4	K	302	-	4,4,4	0.67	0	6,6,6	0.09	0
15	SO4	N	203	-	4,4,4	0.68	0	6,6,6	0.10	0

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.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	N	201	SO4	1	0
15	R	301	SO4	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	249/250 (99%)	1.60	76 (30%) 1 1	18, 38, 73, 97	0
1	O	249/250 (99%)	1.46	64 (25%) 2 2	11, 34, 71, 96	0
2	B	242/258 (93%)	1.94	90 (37%) 1 1	19, 45, 77, 104	0
2	P	244/258 (94%)	1.60	71 (29%) 1 2	15, 35, 73, 97	0
3	C	236/254 (92%)	2.10	110 (46%) 0 1	17, 50, 94, 112	0
3	Q	239/254 (94%)	2.02	106 (44%) 1 1	19, 48, 90, 116	0
4	D	237/260 (91%)	1.74	77 (32%) 1 1	14, 40, 65, 105	0
4	R	239/260 (91%)	2.16	116 (48%) 0 1	20, 52, 79, 103	0
5	E	231/234 (98%)	1.87	86 (37%) 1 1	21, 41, 70, 89	0
5	S	232/234 (99%)	2.25	113 (48%) 0 0	24, 46, 80, 93	0
6	F	244/287 (85%)	1.74	82 (33%) 1 1	18, 39, 75, 83	0
6	T	244/287 (85%)	1.91	86 (35%) 1 1	18, 40, 78, 107	0
7	G	241/252 (95%)	1.48	68 (28%) 1 2	15, 35, 60, 93	0
7	U	242/252 (96%)	1.49	63 (26%) 2 2	15, 35, 62, 92	0
8	H	222/232 (95%)	1.30	45 (20%) 3 4	12, 31, 55, 95	0
8	V	222/232 (95%)	1.16	39 (17%) 4 5	16, 28, 53, 87	0
9	I	204/205 (99%)	1.14	32 (15%) 6 6	14, 29, 55, 80	0
9	W	204/205 (99%)	0.98	21 (10%) 13 13	12, 23, 48, 76	0
10	J	196/198 (98%)	1.03	21 (10%) 12 12	15, 30, 50, 102	0
10	X	195/198 (98%)	1.00	23 (11%) 10 11	12, 27, 52, 106	0
11	K	212/212 (100%)	1.03	19 (8%) 17 15	12, 25, 45, 83	0
11	Y	212/212 (100%)	1.17	35 (16%) 5 6	15, 31, 51, 69	0
12	L	222/222 (100%)	0.91	20 (9%) 17 15	11, 23, 42, 60	0
12	Z	222/222 (100%)	1.27	39 (17%) 4 5	11, 31, 53, 67	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	M	233/233 (100%)	0.97	29 (12%) 9 10	12, 26, 47, 66	0
13	a	233/233 (100%)	1.28	45 (19%) 4 4	15, 30, 52, 74	0
14	N	196/196 (100%)	0.97	23 (11%) 10 11	16, 28, 54, 83	0
14	b	196/196 (100%)	1.01	27 (13%) 8 8	13, 27, 54, 69	0
All	All	6338/6586 (96%)	1.47	1626 (25%) 2 2	11, 34, 72, 116	0

The worst 5 of 1626 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
6	T	40	ASP	7.3
3	Q	241	GLN	7.2
2	P	218	GLY	7.2
5	S	187	GLU	7.2
6	F	244	ASN	7.0

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, 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	SO4	S	301	5/5	0.71	0.36	40,45,49,58	5
15	SO4	Q	301	5/5	0.72	0.28	36,43,48,57	5
15	SO4	K	304	5/5	0.74	0.30	77,93,132,139	0
15	SO4	a	301	5/5	0.74	0.29	43,44,51,68	5
15	SO4	E	301	5/5	0.75	0.26	37,44,50,67	5
15	SO4	M	303	5/5	0.75	0.22	64,65,72,107	0
15	SO4	J	202	5/5	0.75	0.31	40,47,70,79	5

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
15	SO4	T	301	5/5	0.79	0.27	73,86,101,122	0
15	SO4	X	201	5/5	0.79	0.26	31,41,47,65	5
15	SO4	L	303	5/5	0.79	0.32	54,60,108,123	0
15	SO4	a	304	5/5	0.79	0.29	48,65,90,91	0
15	SO4	F	302	5/5	0.80	0.29	64,86,111,139	0
15	SO4	C	301	5/5	0.82	0.18	45,46,57,71	5
15	SO4	Z	303	5/5	0.82	0.28	72,77,103,114	0
16	MG	Z	301	1/1	0.82	0.43	67,67,67,67	0
15	SO4	a	302	5/5	0.83	0.22	30,40,42,55	5
15	SO4	a	303	5/5	0.83	0.22	55,55,70,97	0
15	SO4	J	201	5/5	0.83	0.28	22,26,28,32	5
15	SO4	E	304	5/5	0.83	0.20	43,44,60,80	5
15	SO4	E	303	5/5	0.84	0.19	28,43,56,60	5
15	SO4	K	303	5/5	0.85	0.22	46,48,89,106	0
15	SO4	D	301	5/5	0.86	0.24	55,60,61,85	0
15	SO4	Z	302	5/5	0.86	0.28	66,76,100,119	0
15	SO4	M	301	5/5	0.86	0.22	25,26,48,50	5
15	SO4	F	301	5/5	0.86	0.24	52,57,84,92	0
15	SO4	L	302	5/5	0.87	0.16	38,48,65,92	0
15	SO4	H	302	5/5	0.88	0.22	32,34,40,54	5
15	SO4	S	302	5/5	0.88	0.22	32,33,44,48	5
15	SO4	P	301	5/5	0.88	0.24	33,36,54,60	5
15	SO4	V	302	5/5	0.88	0.24	32,38,42,65	5
15	SO4	N	203	5/5	0.89	0.20	23,35,52,61	5
16	MG	Y	301	1/1	0.89	0.20	29,29,29,29	1
15	SO4	G	301	5/5	0.89	0.19	23,30,59,65	5
15	SO4	I	302	5/5	0.90	0.19	37,41,69,73	5
15	SO4	U	301	5/5	0.90	0.17	41,54,65,105	0
15	SO4	M	302	5/5	0.90	0.23	63,63,93,95	0
15	SO4	P	302	5/5	0.91	0.20	47,66,92,95	0
15	SO4	B	301	5/5	0.91	0.21	46,49,83,97	0
15	SO4	M	304	5/5	0.92	0.24	52,54,57,71	0
15	SO4	G	302	5/5	0.92	0.18	69,69,118,122	0
16	MG	H	301	1/1	0.92	0.16	47,47,47,47	0
15	SO4	E	302	5/5	0.92	0.19	20,23,32,38	5
15	SO4	R	301	5/5	0.92	0.19	37,62,69,80	0
16	MG	L	301	1/1	0.93	0.10	17,17,17,17	0
16	MG	V	301	1/1	0.93	0.18	40,40,40,40	0
15	SO4	b	201	5/5	0.93	0.15	14,17,35,43	5
15	SO4	K	302	5/5	0.93	0.17	28,35,37,41	5
16	MG	W	301	1/1	0.94	0.14	23,23,23,23	0
15	SO4	N	201	5/5	0.94	0.15	18,19,21,29	5

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
16	MG	I	301	1/1	0.94	0.10	27,27,27,27	0
16	MG	K	301	1/1	0.95	0.09	27,27,27,27	0
15	SO4	H	303	5/5	0.95	0.16	36,37,51,53	5
16	MG	N	202	1/1	0.98	0.12	10,10,10,10	0

6.5 Other polymers (i)

There are no such residues in this entry.