wwPDB X-ray Structure Validation Summary Report (i)

Nov 25, 2023 – 10:12 PM EST

PDB ID	:	3NZW
Title	:	Crystal structure of the yeast 20S proteasome in complex with 2b
Authors	:	Groll, M.; Gallastegui, N.; Marechal, X.; Le Ravalec, V.; Basse, N.; Richy, N.; Genin, E.; Huber, R.; Moroder, M.; Vidal, V.; Reboud-Ravaux, M.
Deposited on	:	2010-07-17
Resolution	:	2.50 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 (i)) were used in the production of this report:

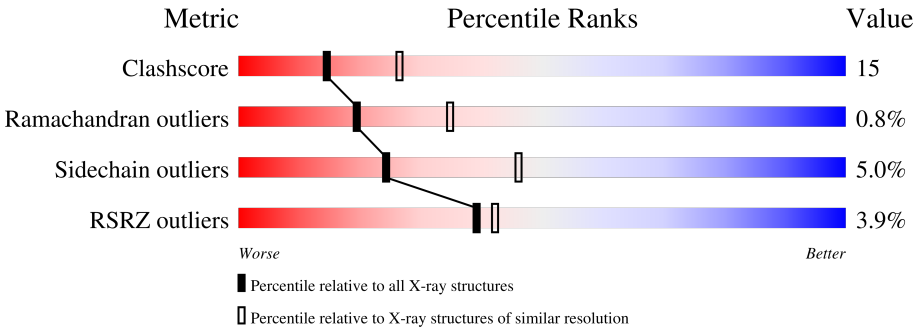
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.50 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))
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	78% 20% ·
1	O	250	3% 79% 18% ·
2	B	258	3% 60% 30% · 5%
2	P	258	6% 61% 29% · 5%
3	C	254	7% 56% 37% · 5%
3	Q	254	19% 57% 36% · 5%

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Mol	Chain	Length	Quality of chain
4	D	260	4% 70% 21% 7%
4	R	260	5% 68% 23% 7%
5	E	234	10% 61% 32% 6%
5	S	234	13% 62% 32% 6%
6	F	288	2% 59% 23% 15%
6	T	288	6% 59% 23% 15%
7	G	252	3% 66% 28%
7	U	252	2% 65% 30%
8	H	261	% 60% 25% 15%
8	V	261	60% 25% 15%
9	I	205	% 74% 24%
9	W	205	% 76% 22%
10	J	198	2% 71% 27%
10	X	198	4% 70% 28%
11	K	287	% 56% 15% 26%
11	Y	287	% 55% 16% 26%
12	L	241	2% 64% 26% 8%
12	Z	241	2% 62% 27% 8%
13	1	266	62% 23% 12%
13	M	266	61% 25% 12%
14	2	215	70% 19% 9%
14	N	215	71% 18% 9%
15	3	5	40% 40% 20%
15	4	5	40% 40% 20%

2 Entry composition (i)

There are 17 unique types of molecules in this entry. The entry contains 51030 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Proteasome component Y7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	250	Total	C	N	O	S	0	0	0
			1915	1219	315	377	4			
1	O	250	Total	C	N	O	S	0	0	0
			1915	1219	315	377	4			

- Molecule 2 is a protein called Proteasome component Y13.

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

- Molecule 3 is a protein called Proteasome component PRE6.

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

- Molecule 4 is a protein called Proteasome component PUP2.

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

- Molecule 5 is a protein called Proteasome component PRE5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	233	Total	C	N	O	S	0	0	0
			1795	1129	312	350	4			
5	S	233	Total	C	N	O	S	0	0	0
			1795	1129	312	350	4			

- Molecule 6 is a protein called Proteasome component C1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	244	Total	C	N	O	S	0	0	0
			1896	1205	330	357	4			
6	T	244	Total	C	N	O	S	0	0	0
			1896	1205	330	357	4			

- Molecule 7 is a protein called Proteasome component C7-alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	243	Total	C	N	O	S	0	0	0
			1921	1221	322	370	8			
7	U	243	Total	C	N	O	S	0	0	0
			1921	1221	322	370	8			

- Molecule 8 is a protein called Proteasome component PUP1.

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

- Molecule 9 is a protein called Proteasome component PUP3.

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

- Molecule 10 is a protein called Proteasome component C11.

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

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

- Molecule 11 is a protein called Proteasome component PRE2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	212	Total	C	N	O	S	0	0	0
			1644	1045	280	312	7			
11	Y	212	Total	C	N	O	S	0	0	0
			1644	1045	280	312	7			

- Molecule 12 is a protein called Proteasome component C5.

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

- Molecule 13 is a protein called Proteasome component PRE4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	233	Total	C	N	O	S	0	0	0
			1824	1154	312	351	7			
13	1	233	Total	C	N	O	S	0	0	0
			1824	1154	312	351	7			

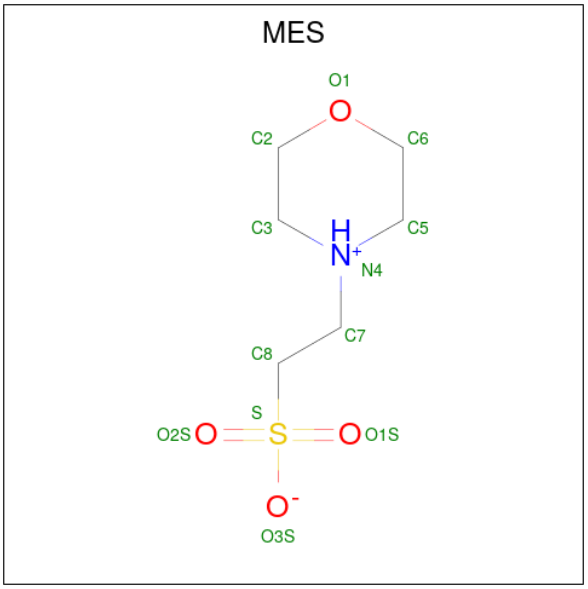
- Molecule 14 is a protein called Proteasome component PRE3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	N	196	Total	C	N	O	S	0	0	0
			1512	955	250	300	7			
14	2	196	Total	C	N	O	S	0	0	0
			1512	955	250	300	7			

- Molecule 15 is a protein called TMC-95A mimic ligand 2b.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	3	5	Total	C	N	O	0	0	0
			55	42	5	8			
15	4	5	Total	C	N	O	0	0	0
			55	42	5	8			

- Molecule 16 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
16	K	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
16	Y	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 17 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	A	58	Total	O	0	0
			58	58		
17	B	37	Total	O	0	0
			37	37		
17	C	43	Total	O	0	0
			43	43		
17	D	37	Total	O	0	0
			37	37		
17	E	23	Total	O	0	0
			23	23		
17	F	48	Total	O	0	0
			48	48		
17	G	64	Total	O	0	0
			64	64		
17	H	51	Total	O	0	0
			51	51		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	I	67	Total O 67 67	0	0
17	J	54	Total O 54 54	0	0
17	K	52	Total O 52 52	0	0
17	L	56	Total O 56 56	0	0
17	M	71	Total O 71 71	0	0
17	N	55	Total O 55 55	0	0
17	O	33	Total O 33 33	0	0
17	P	29	Total O 29 29	0	0
17	Q	27	Total O 27 27	0	0
17	R	29	Total O 29 29	0	0
17	S	22	Total O 22 22	0	0
17	T	39	Total O 39 39	0	0
17	U	60	Total O 60 60	0	0
17	V	47	Total O 47 47	0	0
17	W	64	Total O 64 64	0	0
17	X	50	Total O 50 50	0	0
17	Y	50	Total O 50 50	0	0
17	Z	51	Total O 51 51	0	0
17	1	75	Total O 75 75	0	0
17	2	61	Total O 61 61	0	0
17	3	2	Total O 2 2	0	0

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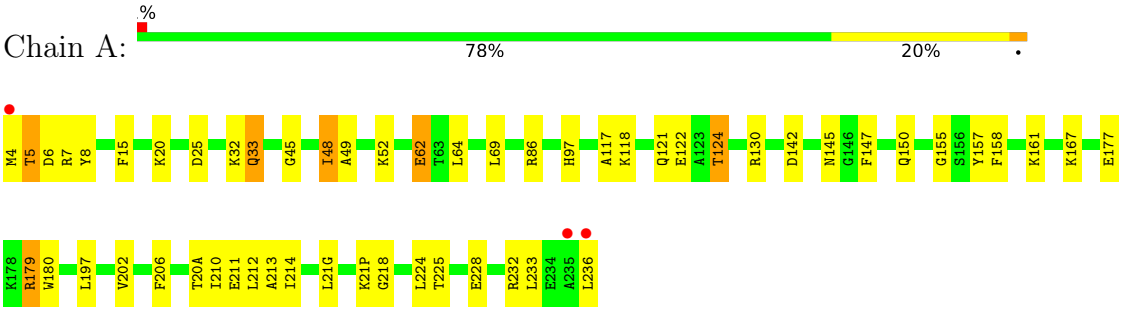
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	4	3	Total O 3 3	0	0

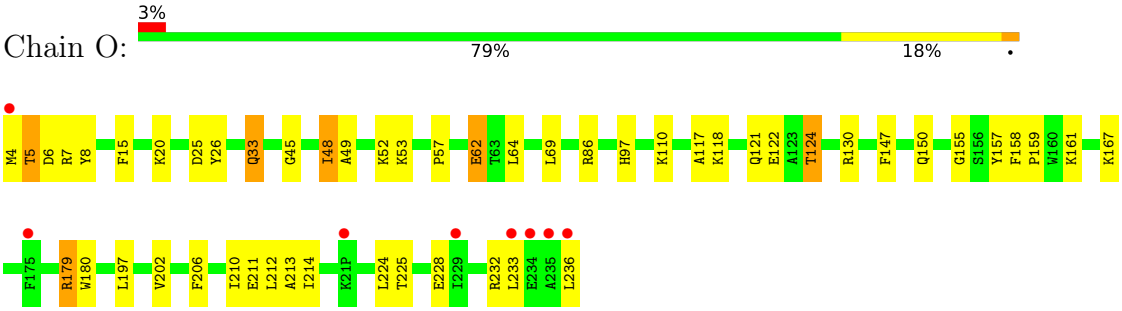
3 Residue-property plots (i)

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

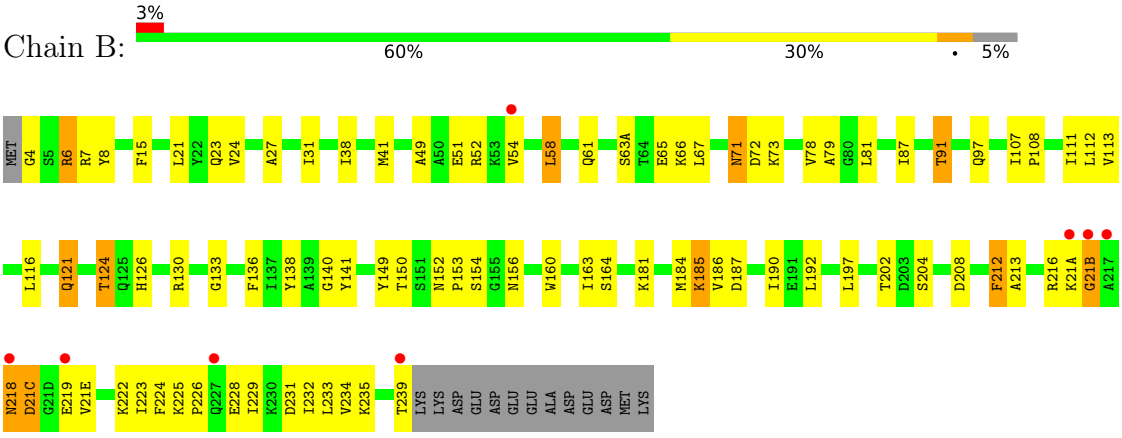
• Molecule 1: Proteasome component Y7



• Molecule 1: Proteasome component Y7

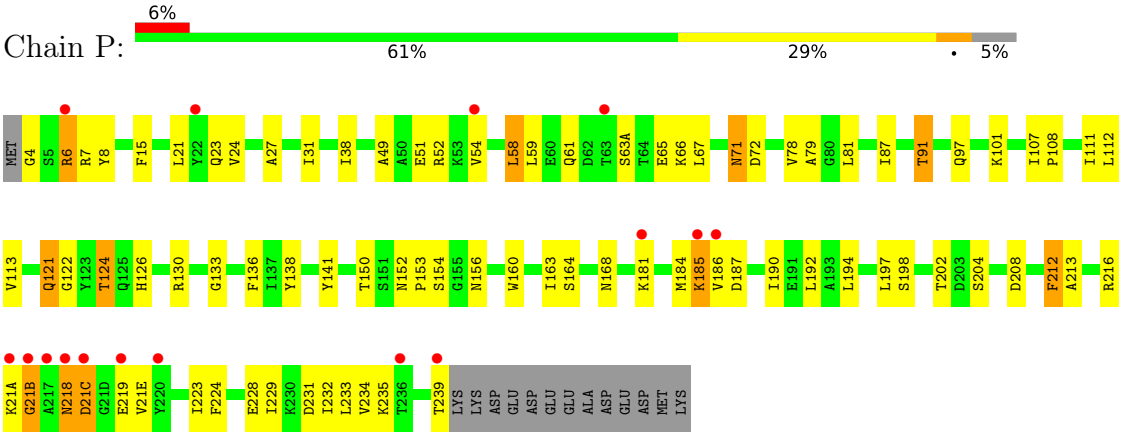


• Molecule 2: Proteasome component Y13



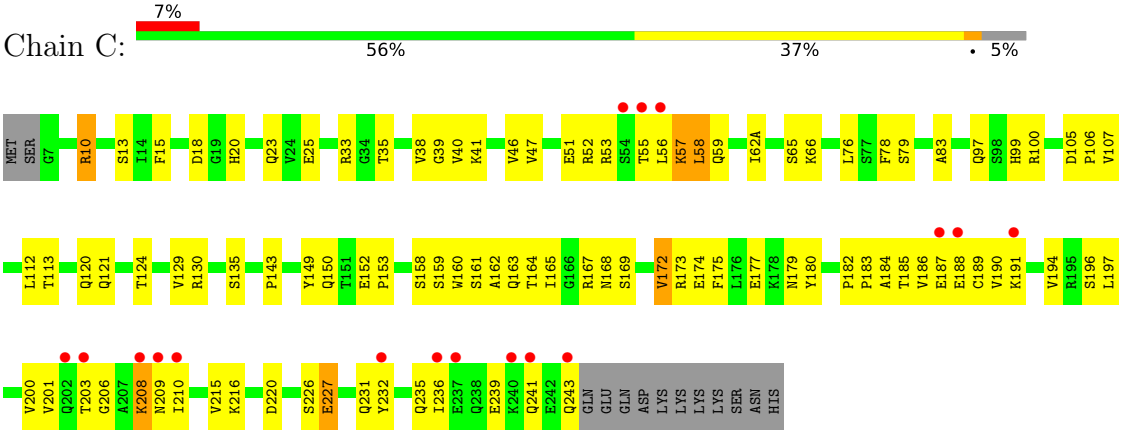
• Molecule 2: Proteasome component Y13

Chain P:



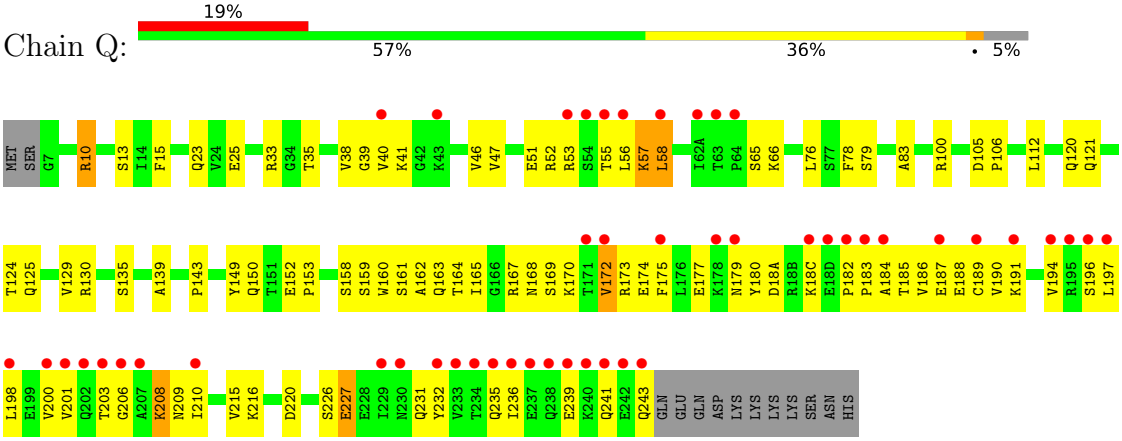
• Molecule 3: Proteasome component PRE6

Chain C:



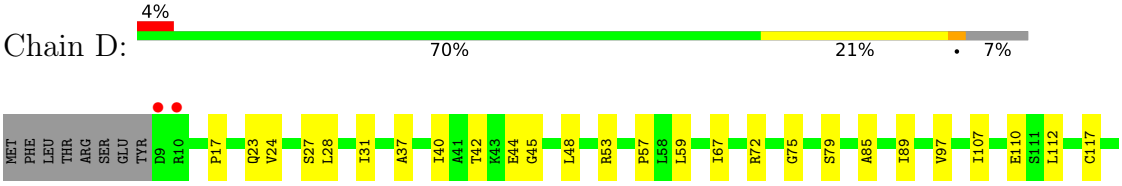
• Molecule 3: Proteasome component PRE6

Chain Q:

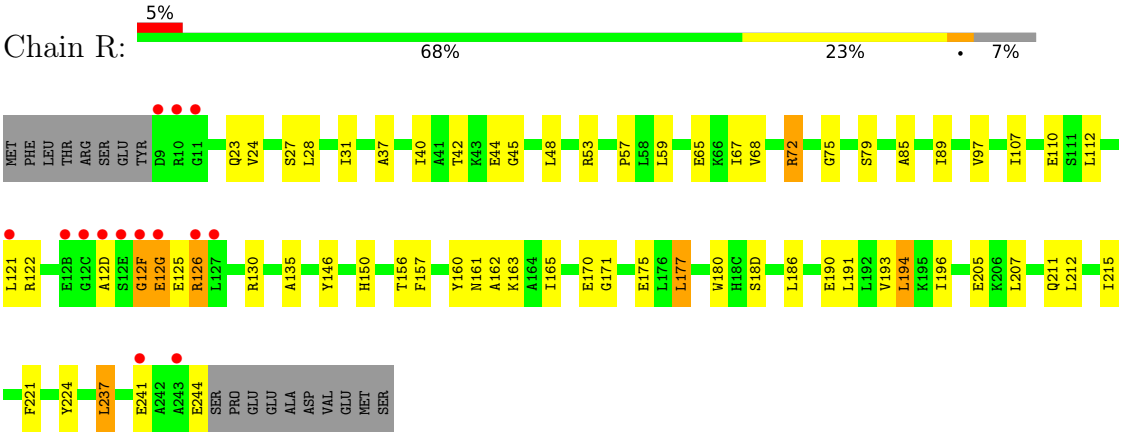


• Molecule 4: Proteasome component PUP2

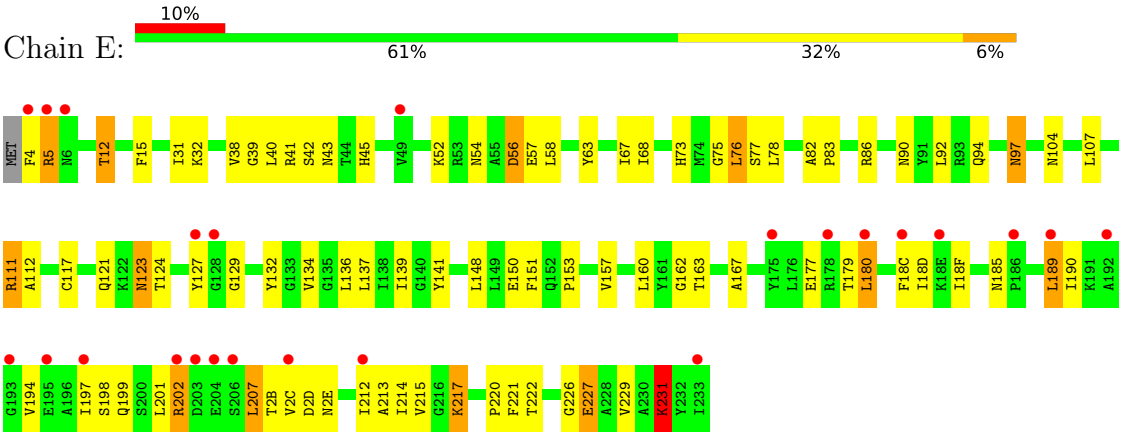
Chain D:



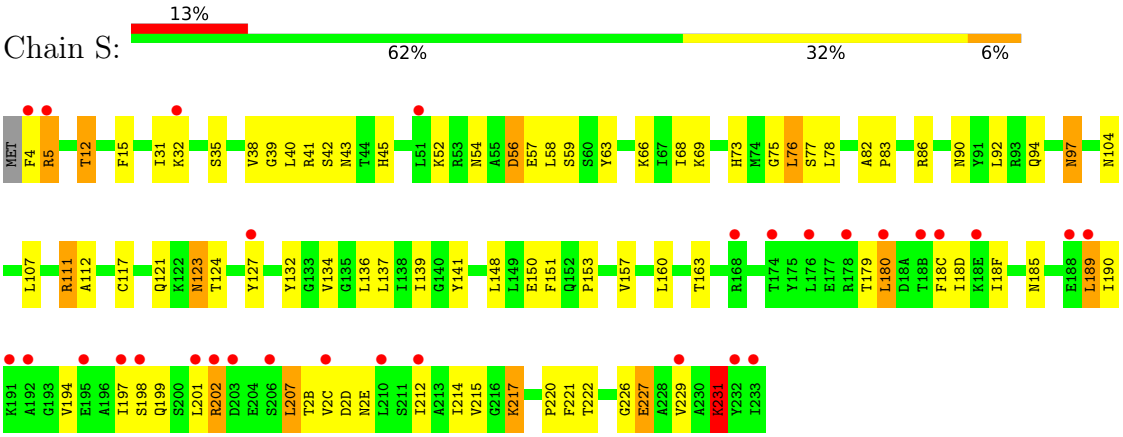
• Molecule 4: Proteasome component PUP2



• Molecule 5: Proteasome component PRE5

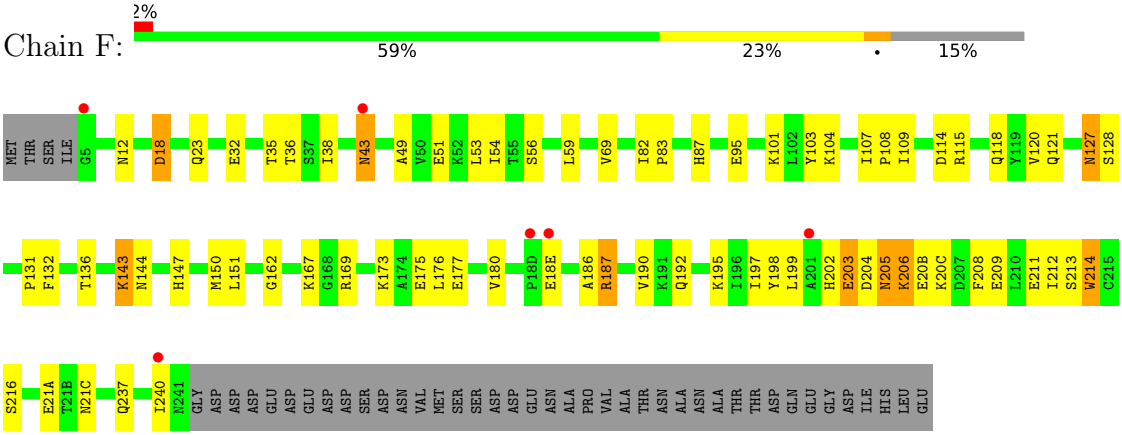


• Molecule 5: Proteasome component PRE5



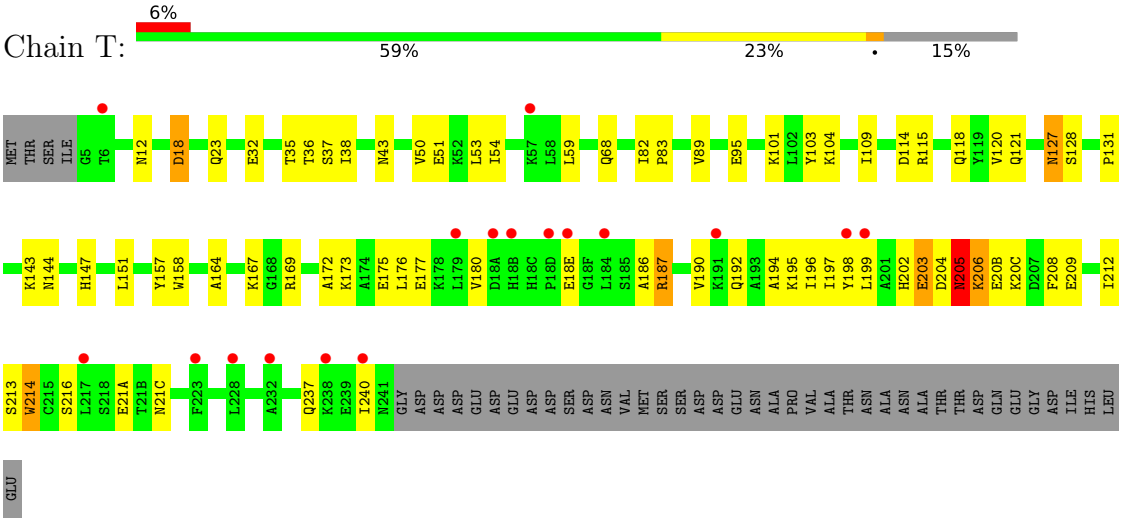
• Molecule 6: Proteasome component C1

Chain F:



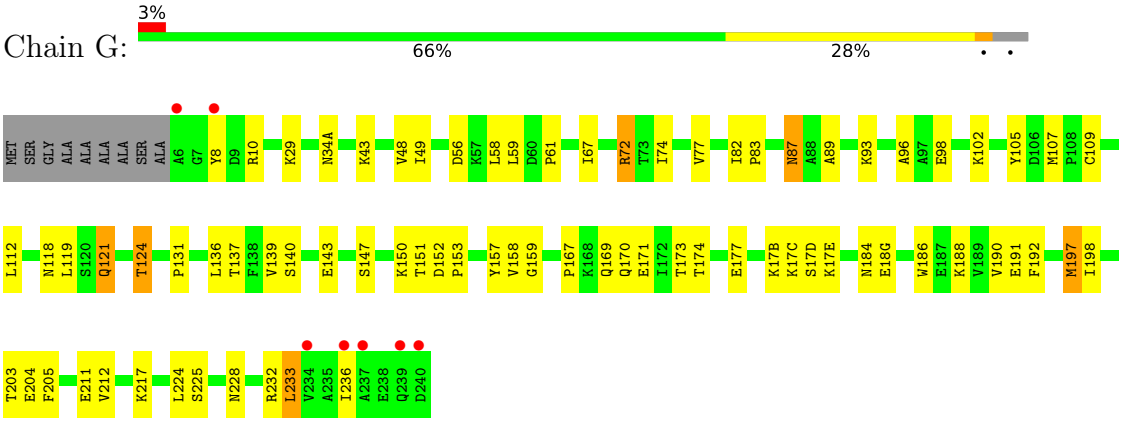
• Molecule 6: Proteasome component C1

Chain T:



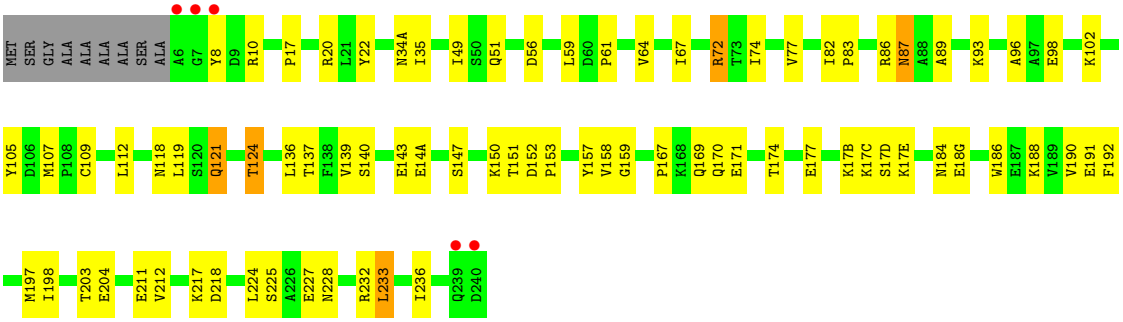
• Molecule 7: Proteasome component C7-alpha

Chain G:

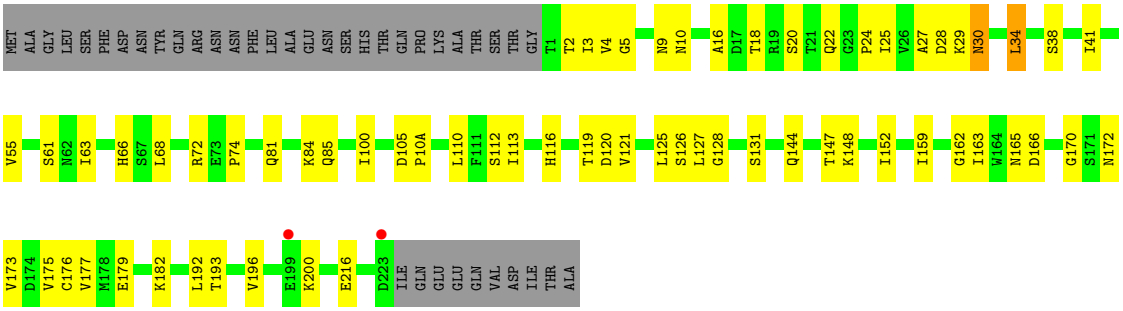


• Molecule 7: Proteasome component C7-alpha

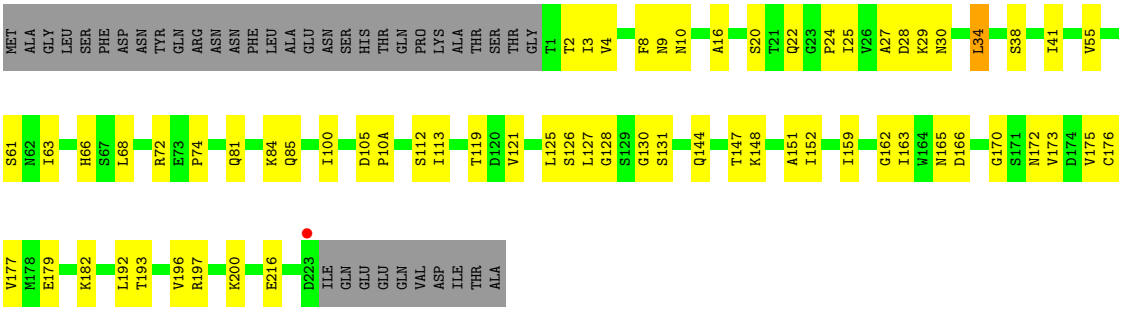
Chain U:



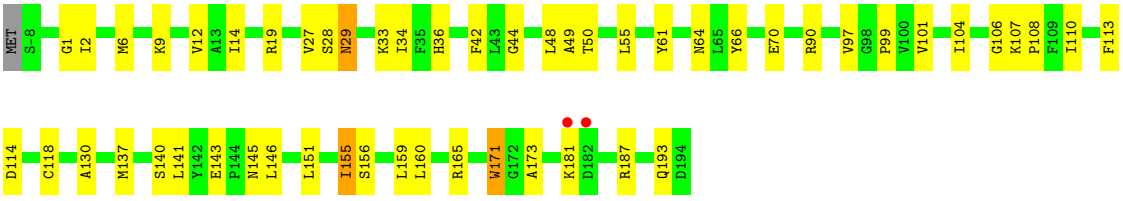
• Molecule 8: Proteasome component PUP1



• Molecule 8: Proteasome component PUP1

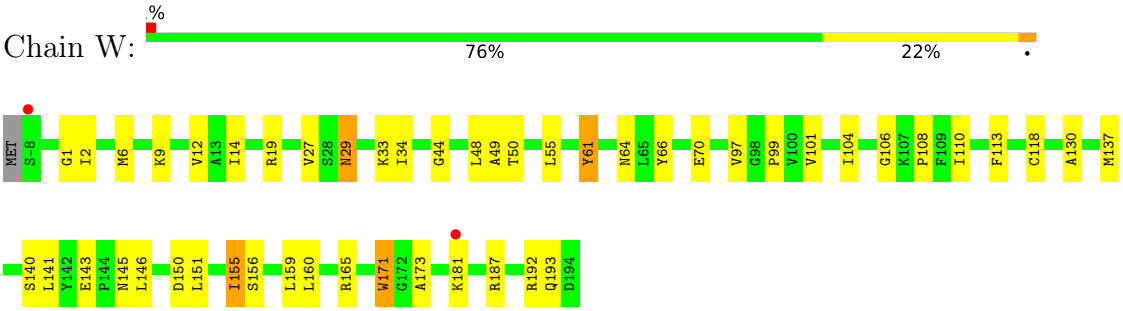


• Molecule 9: Proteasome component PUP3



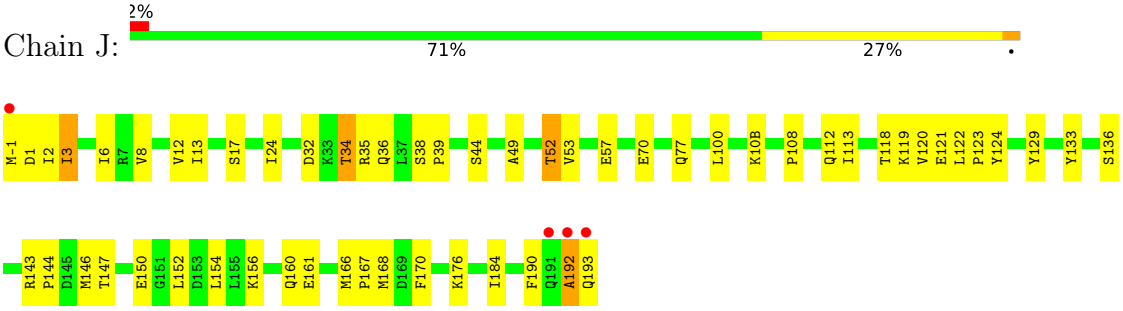
• Molecule 9: Proteasome component PUP3

Chain W:



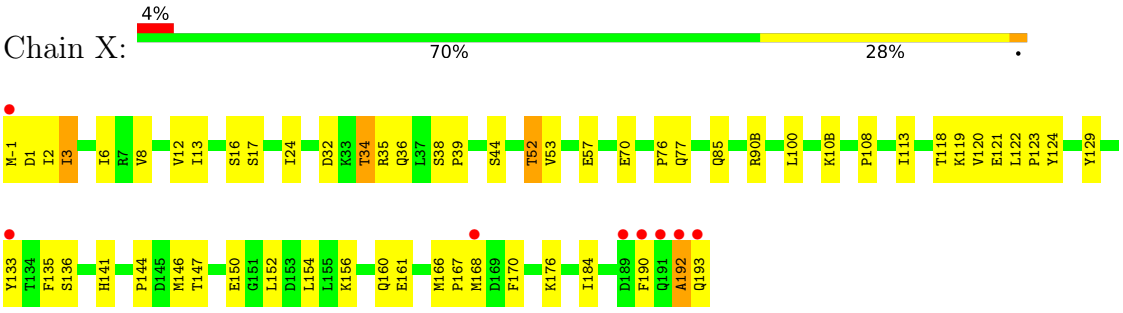
• Molecule 10: Proteasome component C11

Chain J:



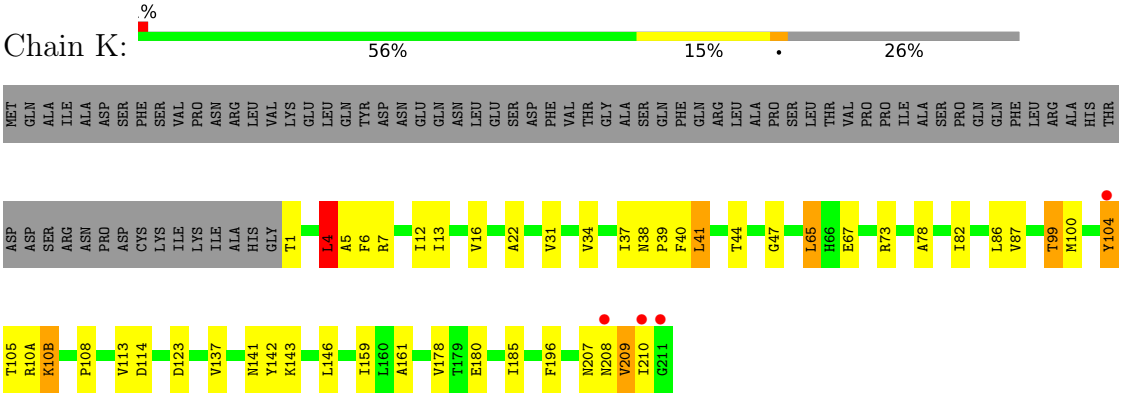
• Molecule 10: Proteasome component C11

Chain X:



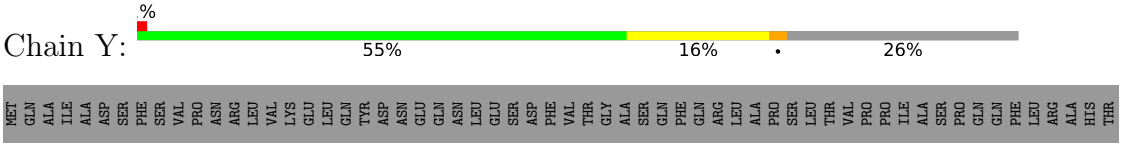
• Molecule 11: Proteasome component PRE2

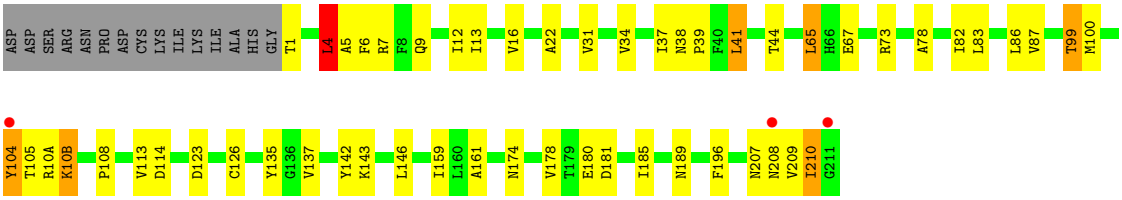
Chain K:



• Molecule 11: Proteasome component PRE2

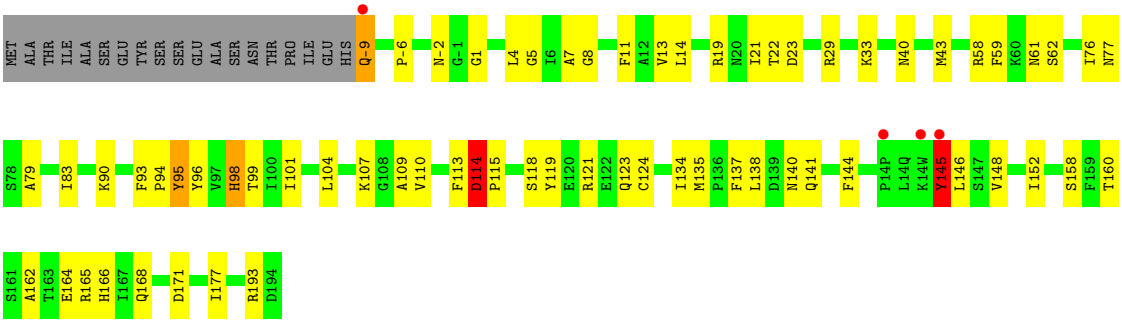
Chain Y:





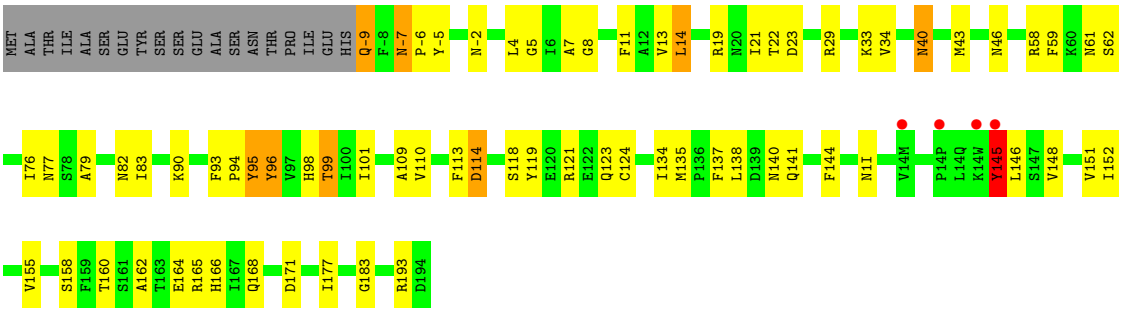
• Molecule 12: Proteasome component C5

Chain L:



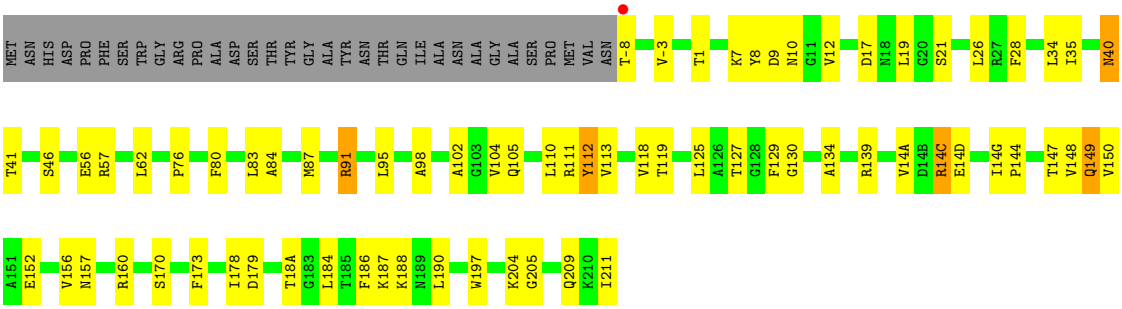
• Molecule 12: Proteasome component C5

Chain Z:



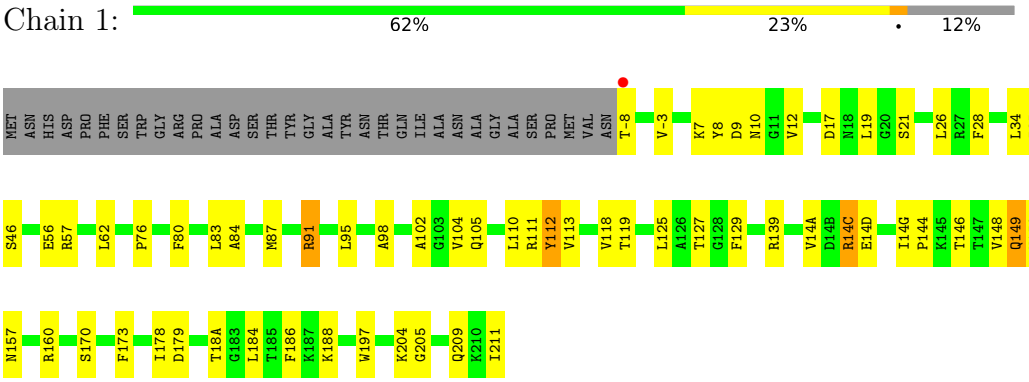
• Molecule 13: Proteasome component PRE4

Chain M:



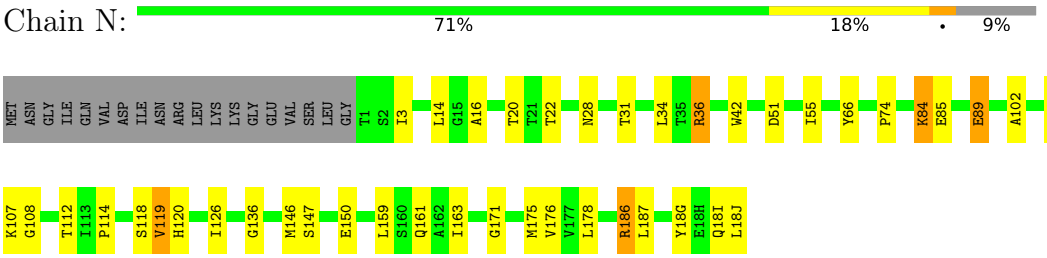
• Molecule 13: Proteasome component PRE4

Chain 1:



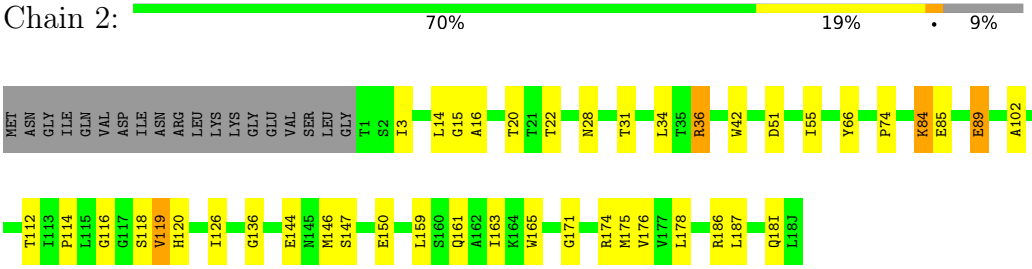
• Molecule 14: Proteasome component PRE3

Chain N:



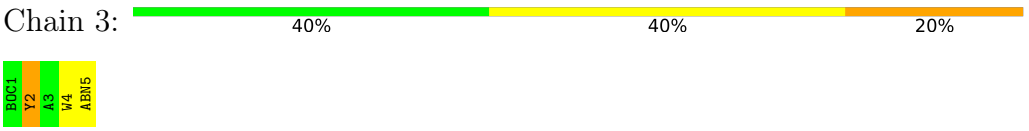
• Molecule 14: Proteasome component PRE3

Chain 2:



• Molecule 15: TMC-95A mimic ligand 2b

Chain 3:



• Molecule 15: TMC-95A mimic ligand 2b

Chain 4:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	135.30Å 300.01Å 144.51Å 90.00° 112.92° 90.00°	Depositor
Resolution (Å)	15.00 – 2.50 49.51 – 2.51	Depositor EDS
% Data completeness (in resolution range)	98.0 (15.00-2.50) 98.0 (49.51-2.51)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.59 (at 2.51Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.219 , 0.240 0.213 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	41.8	Xtriage
Anisotropy	0.870	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 52.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	51030	wwPDB-VP
Average B, all atoms (Å^2)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.05% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: TY5, ABN, RE0, BOC, MES

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	0.36	0/1952	0.62	0/2642
1	O	0.35	0/1952	0.62	0/2642
2	B	0.35	0/1934	0.62	0/2618
2	P	0.36	0/1934	0.62	0/2618
3	C	0.35	0/1919	0.61	0/2598
3	Q	0.33	0/1919	0.61	0/2598
4	D	0.34	0/1886	0.61	0/2541
4	R	0.34	0/1886	0.61	0/2541
5	E	0.34	0/1823	0.58	0/2463
5	S	0.35	0/1823	0.58	0/2463
6	F	0.35	0/1936	0.60	0/2614
6	T	0.36	0/1936	0.61	0/2614
7	G	0.39	0/1959	0.62	0/2652
7	U	0.38	0/1959	0.62	0/2652
8	H	0.37	0/1715	0.66	0/2326
8	V	0.36	0/1715	0.66	0/2326
9	I	0.39	0/1611	0.66	0/2174
9	W	0.39	0/1611	0.67	0/2174
10	J	0.38	0/1613	0.66	0/2173
10	X	0.38	0/1613	0.66	0/2173
11	K	0.45	1/1681 (0.1%)	0.69	2/2274 (0.1%)
11	Y	0.38	0/1681	0.68	2/2274 (0.1%)
12	L	0.38	0/1795	0.70	2/2420 (0.1%)
12	Z	0.37	0/1795	0.68	1/2420 (0.0%)
13	1	0.38	0/1855	0.66	1/2514 (0.0%)
13	M	0.36	0/1855	0.66	1/2514 (0.0%)
14	2	0.38	0/1541	0.64	1/2087 (0.0%)
14	N	0.38	0/1541	0.64	1/2087 (0.0%)
15	3	0.88	0/4	0.73	0/4
15	4	0.91	0/4	0.76	0/4
All	All	0.37	1/50448 (0.0%)	0.64	11/68200 (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
12	L	0	1
12	Z	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	K	47	GLY	C-N	-6.42	1.21	1.33

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	L	114	ASP	O-C-N	-6.93	107.94	121.10
11	K	4	LEU	CA-CB-CG	6.18	129.50	115.30
11	Y	4	LEU	CA-CB-CG	6.07	129.25	115.30
13	1	95	LEU	N-CA-C	-5.71	95.58	111.00
13	M	95	LEU	N-CA-C	-5.60	95.89	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
12	L	145	TYR	Sidechain
12	Z	145	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	1915	0	1926	50	0
1	O	1915	0	1926	50	0
2	B	1904	0	1901	80	0
2	P	1904	0	1901	75	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	1890	0	1900	87	0
3	Q	1890	0	1900	84	0
4	D	1861	0	1836	46	0
4	R	1861	0	1836	50	0
5	E	1795	0	1797	87	0
5	S	1795	0	1797	86	0
6	F	1896	0	1886	60	0
6	T	1896	0	1886	59	0
7	G	1921	0	1910	70	0
7	U	1921	0	1910	78	0
8	H	1684	0	1688	50	0
8	V	1684	0	1688	50	0
9	I	1581	0	1574	47	0
9	W	1581	0	1574	43	0
10	J	1585	0	1590	68	0
10	X	1585	0	1590	80	0
11	K	1644	0	1595	54	0
11	Y	1644	0	1595	56	0
12	L	1757	0	1711	51	0
12	Z	1757	0	1711	57	0
13	1	1824	0	1832	55	0
13	M	1824	0	1832	60	0
14	2	1512	0	1481	38	0
14	N	1512	0	1481	36	0
15	3	55	0	45	4	0
15	4	55	0	45	4	0
16	K	12	0	13	1	0
16	Y	12	0	13	1	0
17	1	75	0	0	2	0
17	2	61	0	0	3	0
17	3	2	0	0	0	0
17	4	3	0	0	0	0
17	A	58	0	0	1	0
17	B	37	0	0	2	0
17	C	43	0	0	2	0
17	D	37	0	0	1	0
17	E	23	0	0	2	0
17	F	48	0	0	3	0
17	G	64	0	0	1	0
17	H	51	0	0	3	0
17	I	67	0	0	4	0
17	J	54	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	K	52	0	0	2	0
17	L	56	0	0	2	0
17	M	71	0	0	2	0
17	N	55	0	0	2	0
17	O	33	0	0	1	0
17	P	29	0	0	1	0
17	Q	27	0	0	3	0
17	R	29	0	0	3	0
17	S	22	0	0	1	0
17	T	39	0	0	1	0
17	U	60	0	0	6	0
17	V	47	0	0	2	0
17	W	64	0	0	3	0
17	X	50	0	0	11	0
17	Y	50	0	0	6	0
17	Z	51	0	0	3	0
All	All	51030	0	49370	1527	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 15.

The worst 5 of 1527 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)
10:J:144:PRO:HG3	11:Y:207:ASN:HD21	1.08	1.14
7:G:96:ALA:HA	7:G:107:MET:HE2	1.34	1.09
11:K:207:ASN:HD21	10:X:144:PRO:HG3	1.11	1.08
11:Y:10(B):LYS:H	11:Y:10(B):LYS:HD2	1.15	1.08
11:K:10(B):LYS:H	11:K:10(B):LYS:HD2	1.15	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	248/250 (99%)	235 (95%)	11 (4%)	2 (1%)	19	35
1	O	248/250 (99%)	236 (95%)	9 (4%)	3 (1%)	13	24
2	B	242/258 (94%)	221 (91%)	17 (7%)	4 (2%)	9	16
2	P	242/258 (94%)	222 (92%)	16 (7%)	4 (2%)	9	16
3	C	239/254 (94%)	223 (93%)	12 (5%)	4 (2%)	9	16
3	Q	239/254 (94%)	224 (94%)	11 (5%)	4 (2%)	9	16
4	D	240/260 (92%)	225 (94%)	12 (5%)	3 (1%)	12	21
4	R	240/260 (92%)	225 (94%)	12 (5%)	3 (1%)	12	21
5	E	231/234 (99%)	210 (91%)	16 (7%)	5 (2%)	6	10
5	S	231/234 (99%)	208 (90%)	18 (8%)	5 (2%)	6	10
6	F	242/288 (84%)	231 (96%)	8 (3%)	3 (1%)	13	24
6	T	242/288 (84%)	230 (95%)	9 (4%)	3 (1%)	13	24
7	G	241/252 (96%)	228 (95%)	13 (5%)	0	100	100
7	U	241/252 (96%)	227 (94%)	14 (6%)	0	100	100
8	H	220/261 (84%)	209 (95%)	11 (5%)	0	100	100
8	V	220/261 (84%)	209 (95%)	11 (5%)	0	100	100
9	I	202/205 (98%)	196 (97%)	6 (3%)	0	100	100
9	W	202/205 (98%)	196 (97%)	6 (3%)	0	100	100
10	J	196/198 (99%)	185 (94%)	8 (4%)	3 (2%)	10	18
10	X	196/198 (99%)	186 (95%)	8 (4%)	2 (1%)	15	28
11	K	210/287 (73%)	203 (97%)	6 (3%)	1 (0%)	29	48
11	Y	210/287 (73%)	202 (96%)	7 (3%)	1 (0%)	29	48
12	L	220/241 (91%)	208 (94%)	12 (6%)	0	100	100
12	Z	220/241 (91%)	208 (94%)	12 (6%)	0	100	100
13	1	231/266 (87%)	221 (96%)	10 (4%)	0	100	100
13	M	231/266 (87%)	221 (96%)	10 (4%)	0	100	100
14	2	194/215 (90%)	186 (96%)	8 (4%)	0	100	100
14	N	194/215 (90%)	185 (95%)	9 (5%)	0	100	100
15	3	1/5 (20%)	1 (100%)	0	0	100	100
15	4	1/5 (20%)	1 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	6314/6948 (91%)	5962 (94%)	302 (5%)	50 (1%)	19 35

5 of 50 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	21(C)	ASP
3	C	58	LEU
3	C	203	THR
4	D	12(G)	GLU
5	E	5	ARG

5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	209/209 (100%)	200 (96%)	9 (4%)	29 53
1	O	209/209 (100%)	201 (96%)	8 (4%)	33 58
2	B	203/216 (94%)	192 (95%)	11 (5%)	22 42
2	P	203/216 (94%)	192 (95%)	11 (5%)	22 42
3	C	213/226 (94%)	203 (95%)	10 (5%)	26 49
3	Q	213/226 (94%)	203 (95%)	10 (5%)	26 49
4	D	198/215 (92%)	186 (94%)	12 (6%)	18 36
4	R	198/215 (92%)	186 (94%)	12 (6%)	18 36
5	E	192/193 (100%)	175 (91%)	17 (9%)	9 19
5	S	192/193 (100%)	175 (91%)	17 (9%)	9 19
6	F	201/239 (84%)	188 (94%)	13 (6%)	17 33
6	T	201/239 (84%)	188 (94%)	13 (6%)	17 33
7	G	207/210 (99%)	197 (95%)	10 (5%)	25 48
7	U	207/210 (99%)	197 (95%)	10 (5%)	25 48
8	H	181/214 (85%)	175 (97%)	6 (3%)	38 64
8	V	181/214 (85%)	174 (96%)	7 (4%)	32 57

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	I	172/173 (99%)	167 (97%)	5 (3%)	42	69
9	W	172/173 (99%)	167 (97%)	5 (3%)	42	69
10	J	175/175 (100%)	169 (97%)	6 (3%)	37	63
10	X	175/175 (100%)	169 (97%)	6 (3%)	37	63
11	K	169/235 (72%)	160 (95%)	9 (5%)	22	43
11	Y	169/235 (72%)	159 (94%)	10 (6%)	19	37
12	L	185/201 (92%)	177 (96%)	8 (4%)	29	53
12	Z	185/201 (92%)	173 (94%)	12 (6%)	17	33
13	1	199/224 (89%)	191 (96%)	8 (4%)	31	56
13	M	199/224 (89%)	191 (96%)	8 (4%)	31	56
14	2	162/178 (91%)	154 (95%)	8 (5%)	25	47
14	N	162/178 (91%)	154 (95%)	8 (5%)	25	47
All	All	5332/5816 (92%)	5063 (95%)	269 (5%)	24	46

5 of 269 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
11	Y	4	LEU
11	Y	10(B)	LYS
13	1	204	LYS
10	J	77	GLN
10	J	34	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 184 such sidechains are listed below:

Mol	Chain	Res	Type
5	S	64	GLN
8	V	144	GLN
5	S	123	ASN
6	T	192	GLN
10	X	62	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

4 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
15	TY5	3	2	15	19,20,21	1.73	3 (15%)	22,25,27	0.95	1 (4%)
15	TY5	4	2	15	19,20,21	1.73	5 (26%)	22,25,27	0.92	1 (4%)
15	RE0	4	4	15	15,17,18	1.39	2 (13%)	19,25,27	2.29	7 (36%)
15	RE0	3	4	15	15,17,18	1.28	1 (6%)	19,25,27	2.46	7 (36%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	TY5	3	2	15	-	0/10/11/13	0/2/2/2
15	TY5	4	2	15	-	0/10/11/13	0/2/2/2
15	RE0	4	4	15	-	0/6/23/25	0/2/2/2
15	RE0	3	4	15	-	0/6/23/25	0/2/2/2

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	3	2	TY5	CE2-CZ	2.85	1.44	1.38
15	4	2	TY5	CE2-CZ	2.65	1.43	1.38
15	4	4	RE0	CB-CA	2.49	1.57	1.54
15	4	2	TY5	C49-C50	2.44	1.56	1.50
15	4	2	TY5	C55-C50	2.21	1.43	1.38

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	3	4	RE0	CG-CD2-CE2	-7.20	105.97	108.86
15	4	4	RE0	CG-CD2-CE2	-6.49	106.25	108.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	4	4	RE0	CD2-CE2-NE1	3.68	112.06	109.59
15	3	4	RE0	CD2-CE2-NE1	3.49	111.93	109.59
15	4	4	RE0	CE2-NE1-CD1	-3.14	109.98	111.86

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	3	2	TY5	2	0
15	4	2	TY5	2	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
16	MES	Y	212	-	12,12,12	2.43	5 (41%)	14,16,16	2.06	4 (28%)
16	MES	K	212	-	12,12,12	1.07	0	14,16,16	0.82	0

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
16	MES	Y	212	-	-	1/6/14/14	0/1/1/1
16	MES	K	212	-	-	4/6/14/14	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	Y	212	MES	O2S-S	4.52	1.58	1.45
16	Y	212	MES	C7-N4	3.67	1.55	1.47
16	Y	212	MES	C8-S	3.50	1.82	1.77
16	Y	212	MES	C3-N4	2.94	1.55	1.46
16	Y	212	MES	C5-N4	2.90	1.54	1.46

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	Y	212	MES	O3S-S-O1S	4.69	122.72	111.27
16	Y	212	MES	C6-C5-N4	-3.81	104.32	110.10
16	Y	212	MES	O3S-S-O2S	-2.79	104.46	111.27
16	Y	212	MES	C2-C3-N4	2.56	113.99	110.10

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
16	K	212	MES	C8-C7-N4-C3
16	Y	212	MES	C8-C7-N4-C3
16	K	212	MES	C7-C8-S-O3S
16	K	212	MES	C7-C8-S-O1S
16	K	212	MES	C7-C8-S-O2S

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	Y	212	MES	1	0
16	K	212	MES	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	250/250 (100%)	-0.13	3 (1%) 79 80	33, 46, 75, 104	0
1	O	250/250 (100%)	0.02	8 (3%) 47 51	37, 53, 81, 104	0
2	B	244/258 (94%)	0.09	8 (3%) 46 50	32, 52, 89, 116	0
2	P	244/258 (94%)	0.18	16 (6%) 18 19	34, 53, 90, 116	0
3	C	241/254 (94%)	0.21	17 (7%) 16 16	33, 55, 107, 120	0
3	Q	241/254 (94%)	0.72	49 (20%) 1 0	38, 60, 111, 122	0
4	D	242/260 (93%)	0.13	10 (4%) 37 40	34, 54, 89, 120	0
4	R	242/260 (93%)	0.26	14 (5%) 23 24	37, 58, 90, 122	0
5	E	233/234 (99%)	0.34	24 (10%) 6 6	43, 59, 85, 110	0
5	S	233/234 (99%)	0.66	30 (12%) 3 3	41, 64, 90, 108	0
6	F	244/288 (84%)	0.01	6 (2%) 57 61	36, 53, 88, 103	0
6	T	244/288 (84%)	0.20	17 (6%) 16 16	32, 55, 92, 106	0
7	G	243/252 (96%)	-0.08	7 (2%) 51 55	33, 46, 76, 113	0
7	U	243/252 (96%)	-0.03	5 (2%) 63 66	32, 50, 74, 113	0
8	H	222/261 (85%)	-0.21	2 (0%) 84 86	28, 45, 65, 90	0
8	V	222/261 (85%)	-0.24	1 (0%) 91 91	30, 49, 67, 93	0
9	I	204/205 (99%)	-0.19	2 (0%) 82 84	28, 43, 62, 76	0
9	W	204/205 (99%)	-0.09	2 (0%) 82 84	31, 44, 64, 78	0
10	J	198/198 (100%)	-0.13	4 (2%) 65 68	29, 43, 64, 120	0
10	X	198/198 (100%)	-0.12	8 (4%) 38 41	29, 45, 62, 120	0
11	K	212/287 (73%)	-0.21	4 (1%) 66 69	26, 42, 65, 78	0
11	Y	212/287 (73%)	-0.10	3 (1%) 75 77	33, 46, 68, 79	0
12	L	222/241 (92%)	-0.14	4 (1%) 68 71	29, 46, 66, 91	0
12	Z	222/241 (92%)	-0.10	4 (1%) 68 71	31, 46, 67, 93	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	1	233/266 (87%)	-0.31	1 (0%) 92 93	31, 45, 59, 64	0
13	M	233/266 (87%)	-0.27	1 (0%) 92 93	30, 47, 61, 65	0
14	2	196/215 (91%)	-0.20	1 (0%) 91 91	27, 44, 66, 80	0
14	N	196/215 (91%)	-0.35	0 100 100	32, 43, 64, 76	0
15	3	1/5 (20%)	-0.81	0 100 100	33, 33, 33, 33	0
15	4	1/5 (20%)	0.20	0 100 100	43, 43, 43, 43	0
All	All	6370/6948 (91%)	0.01	251 (3%) 39 42	26, 49, 82, 122	0

The worst 5 of 251 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	D	12(C)	GLY	12.6
3	C	55	THR	11.1
4	R	12(D)	ALA	11.0
4	D	12(D)	ALA	10.8
7	U	6	ALA	10.3

6.2 Non-standard residues in protein, DNA, RNA chains (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	TY5	3	2	19/20	0.94	0.15	37,40,47,47	0
15	TY5	4	2	19/20	0.94	0.13	33,41,44,44	0
15	RE0	3	4	16/17	0.95	0.18	34,36,39,46	0
15	RE0	4	4	16/17	0.95	0.14	41,43,44,49	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95^{th} 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
16	MES	Y	212	12/12	0.96	0.23	59,62,64,64	0
16	MES	K	212	12/12	0.98	0.18	48,54,56,57	0

6.5 Other polymers (i)

There are no such residues in this entry.