wwPDB X-ray Structure Validation Summary Report (i)

Feb 1, 2016 – 11:10 AM GMT

PDB ID	:	3NZJ
Title	:	Crystal structure of yeast 20S proteasome in complex with ligand 2a
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	:	2010-07-16
Resolution	:	2.40 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

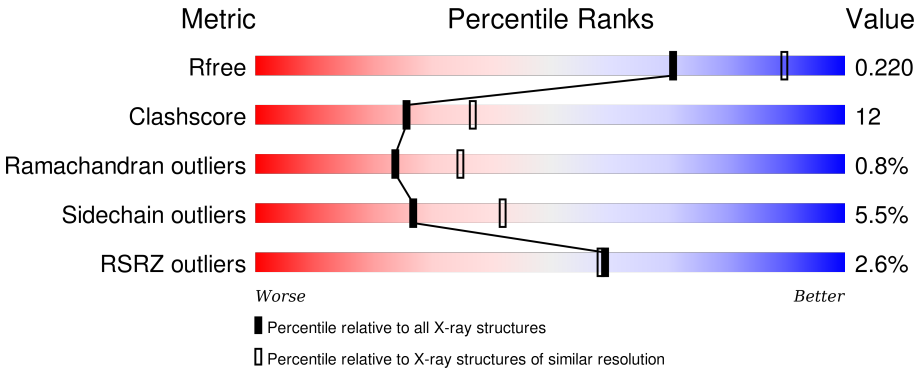
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.40 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}	91344	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (2.40-2.40)

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 on the lower 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% 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	2% 82% 17% •
1	O	250	2% 80% 19% •
2	B	258	2% 71% 19% • 5%
2	P	258	4% 71% 20% • 5%
3	C	254	4% 64% 27% • 5%

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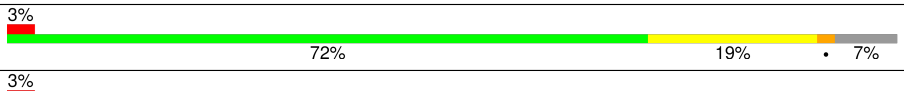
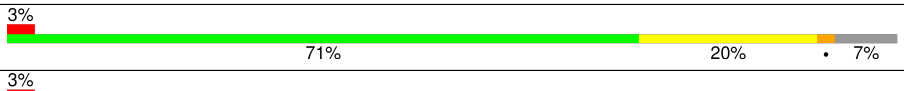
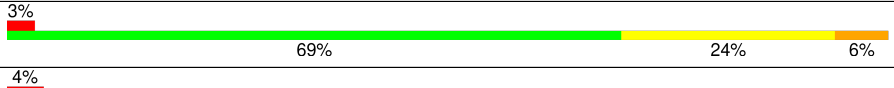
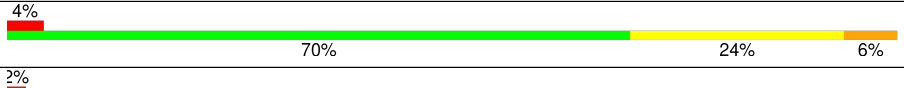
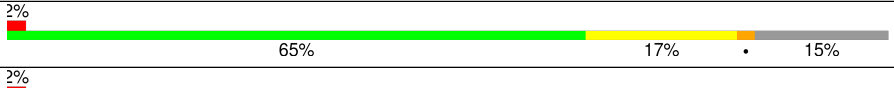
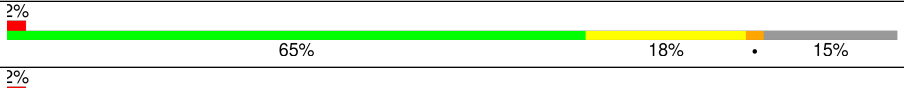
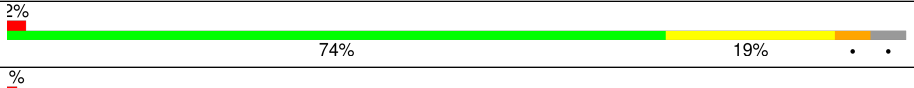
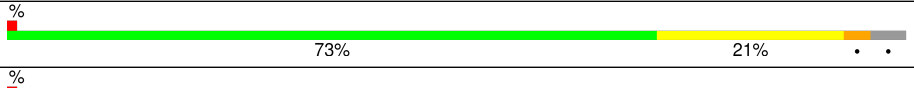
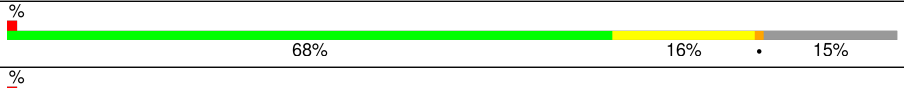
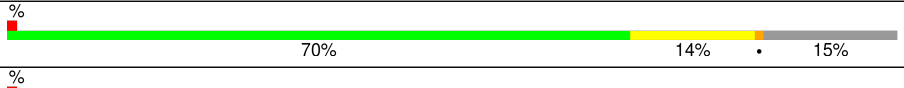
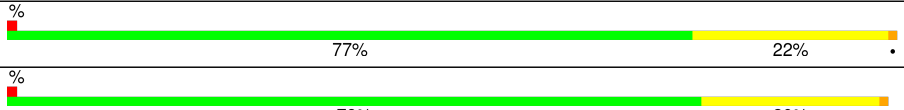
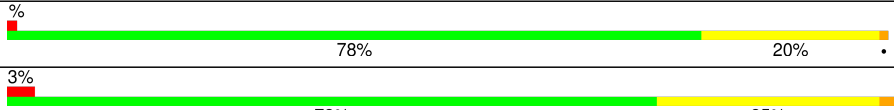
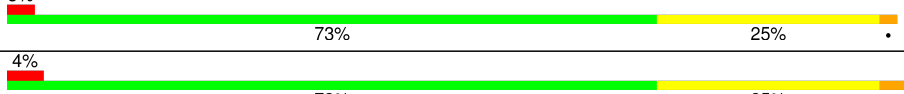
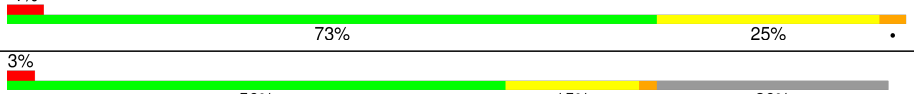
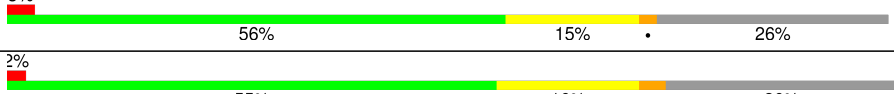
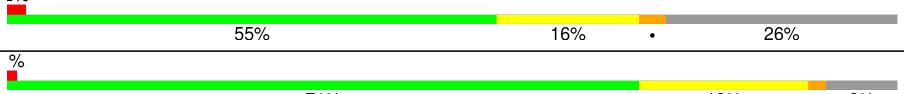
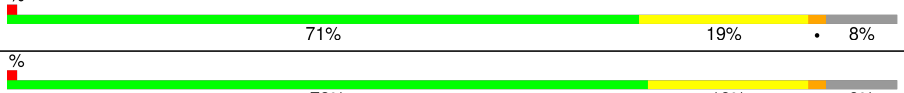
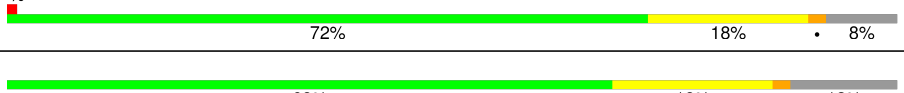
Mol	Chain	Length	Quality of chain
3	Q	254	
4	D	260	
4	R	260	
5	E	234	
5	S	234	
6	F	288	
6	T	288	
7	G	252	
7	U	252	
8	H	261	
8	V	261	
9	I	205	
9	W	205	
10	J	198	
10	X	198	
11	K	287	
11	Y	287	
12	L	241	
12	Z	241	
13	1	266	
13	M	266	
14	2	215	
14	N	215	
15	3	5	
15	4	5	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
16	MES	K	212	-	-	-	X

2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 51006 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			

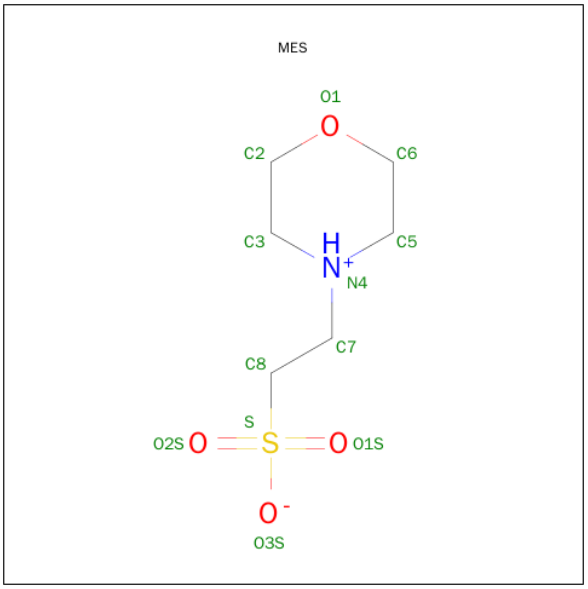
- Molecule 14 is a protein called Proteasome component PRE3.

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 2a.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	3	5	Total	C	N	O	0	0	0
			54	42	5	7			
15	4	5	Total	C	N	O	0	0	0
			54	42	5	7			

- 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	39	Total	O	0	0
			39	39		
17	C	43	Total	O	0	0
			43	43		
17	D	38	Total	O	0	0
			38	38		
17	E	22	Total	O	0	0
			22	22		
17	F	48	Total	O	0	0
			48	48		
17	G	62	Total	O	0	0
			62	62		
17	H	51	Total	O	0	0
			51	51		

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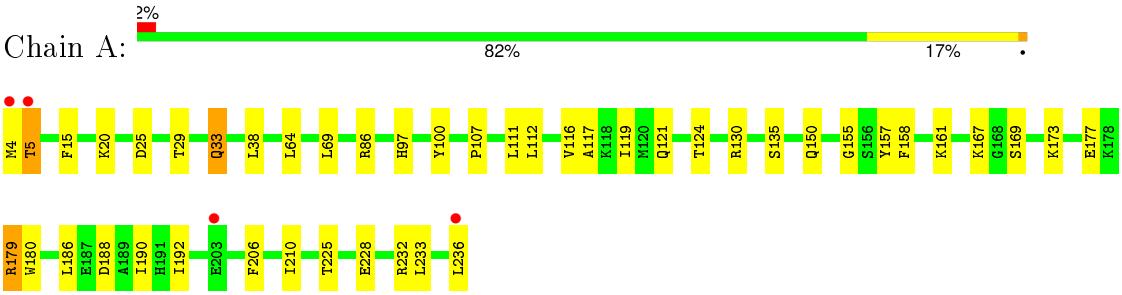
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	I	65	Total O 65 65	0	0
17	J	52	Total O 52 52	0	0
17	K	42	Total O 42 42	0	0
17	L	57	Total O 57 57	0	0
17	M	71	Total O 71 71	0	0
17	N	61	Total O 61 61	0	0
17	O	33	Total O 33 33	0	0
17	P	30	Total O 30 30	0	0
17	Q	26	Total O 26 26	0	0
17	R	31	Total O 31 31	0	0
17	S	19	Total O 19 19	0	0
17	T	40	Total O 40 40	0	0
17	U	61	Total O 61 61	0	0
17	V	49	Total O 49 49	0	0
17	W	61	Total O 61 61	0	0
17	X	48	Total O 48 48	0	0
17	Y	48	Total O 48 48	0	0
17	Z	51	Total O 51 51	0	0
17	1	70	Total O 70 70	0	0
17	2	60	Total O 60 60	0	0

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 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.

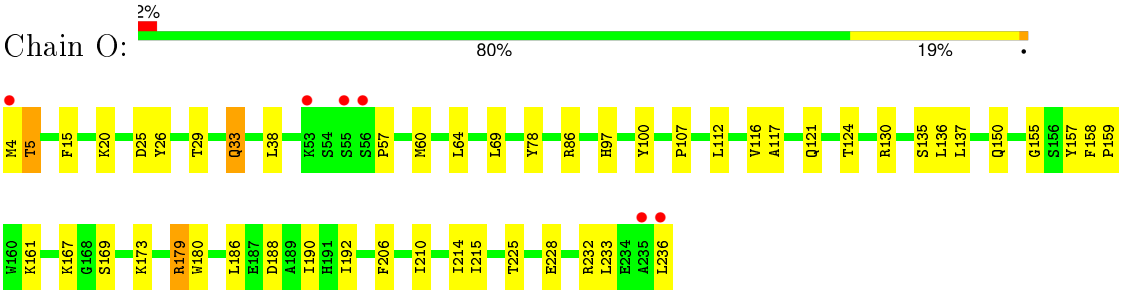
- Molecule 1: Proteasome component Y7

Chain A:



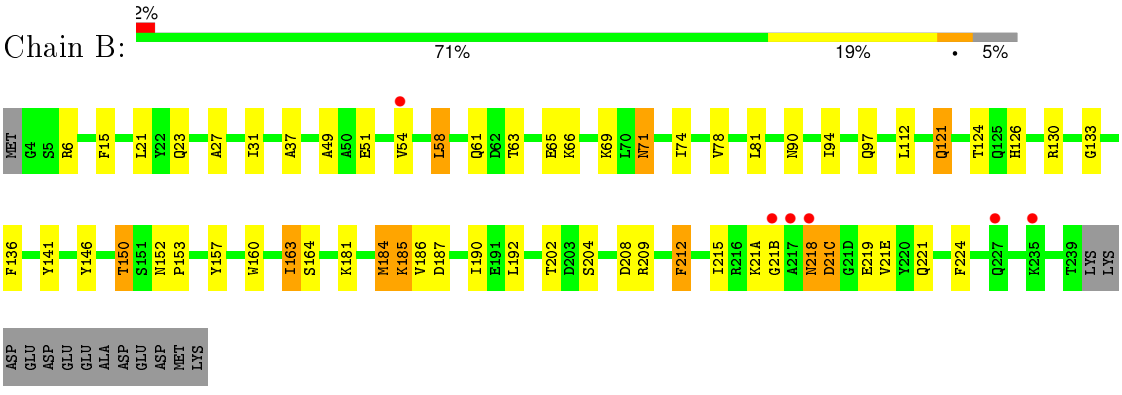
- Molecule 1: Proteasome component Y7

Chain O:



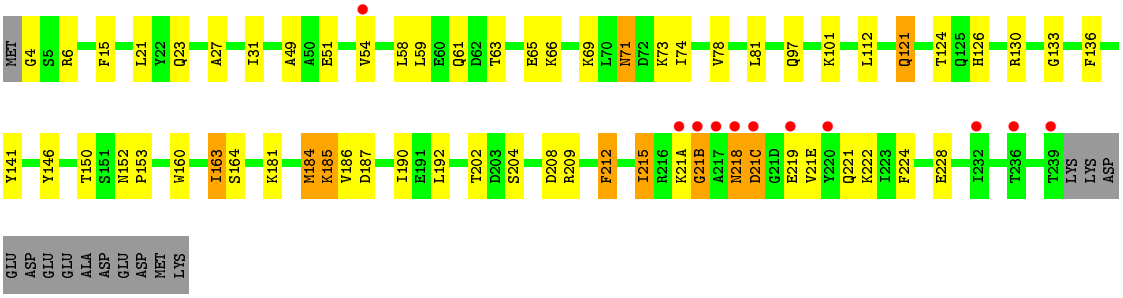
- Molecule 2: Proteasome component Y13

Chain B:

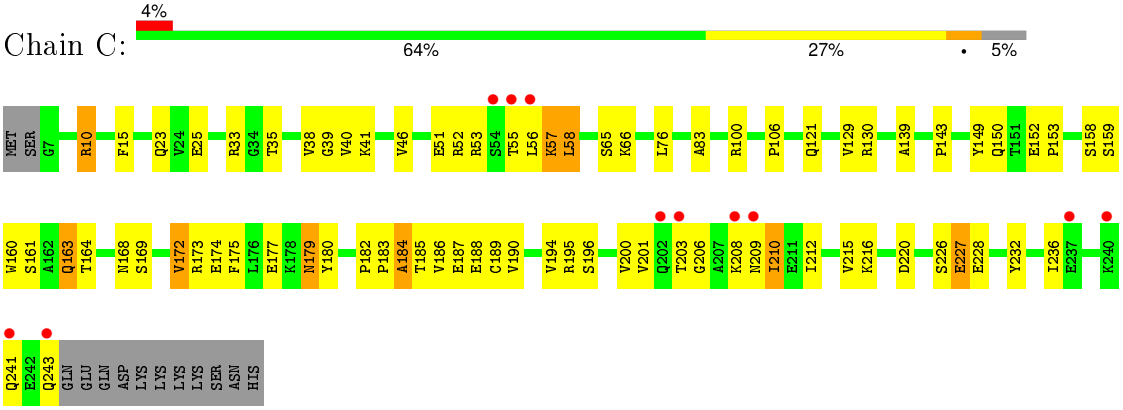


- Molecule 2: Proteasome component Y13

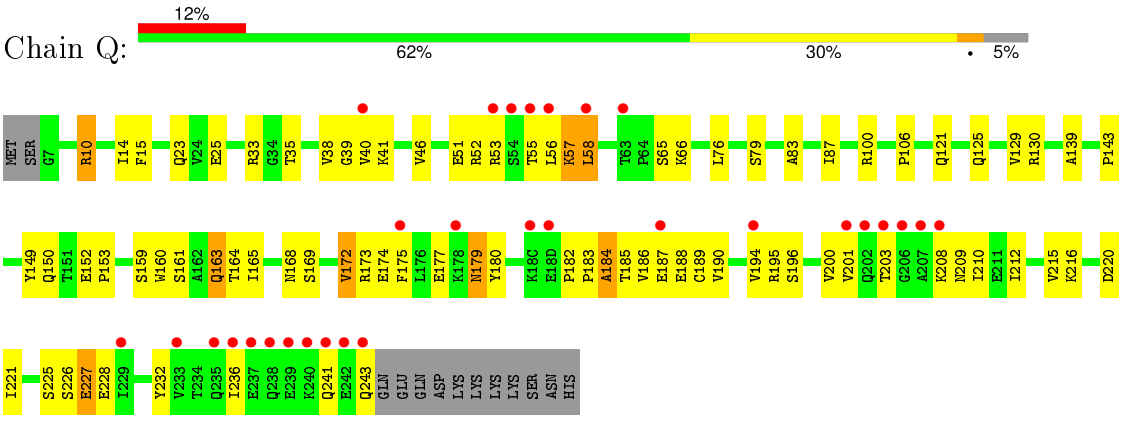
Chain P:



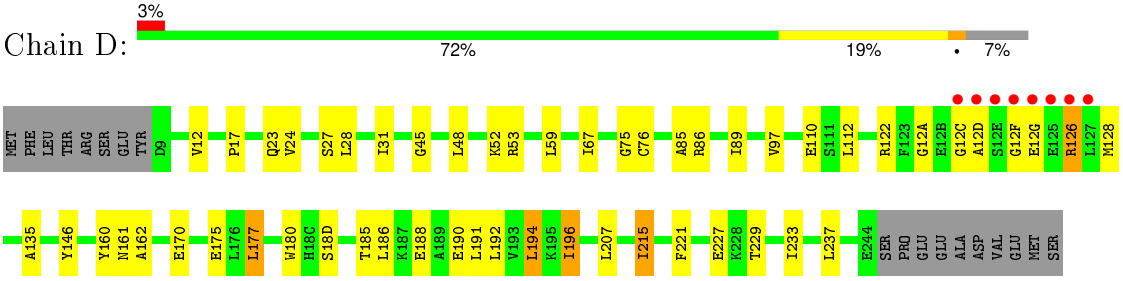
• Molecule 3: Proteasome component PRE6



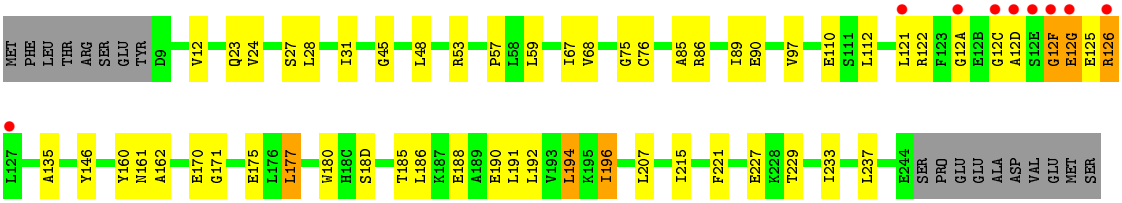
• Molecule 3: Proteasome component PRE6



• Molecule 4: Proteasome component PUP2

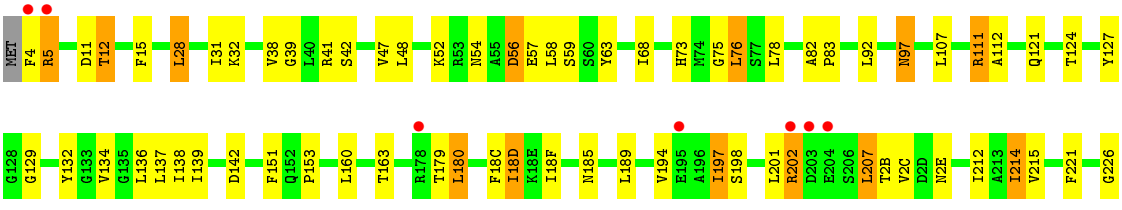


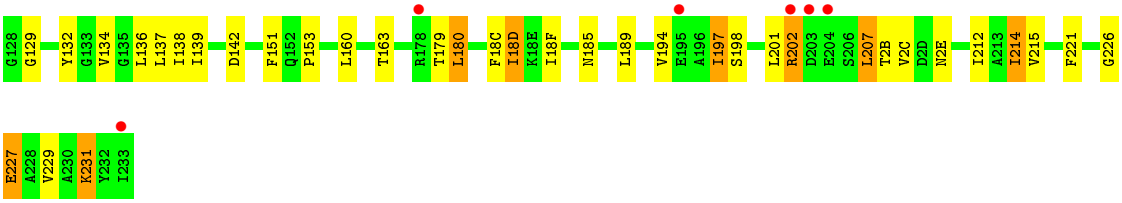
• Molecule 4: Proteasome component PUP2



• Molecule 5: Proteasome component PRE5

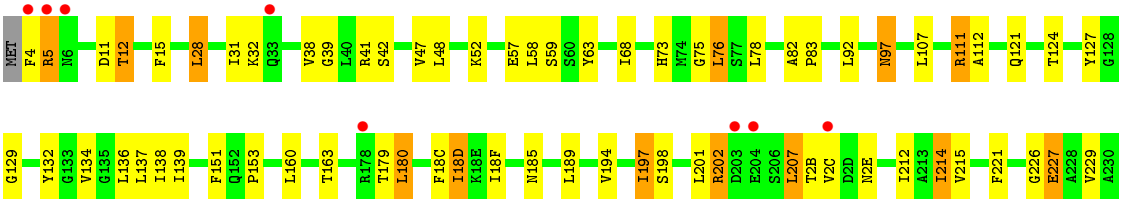
Chain E:

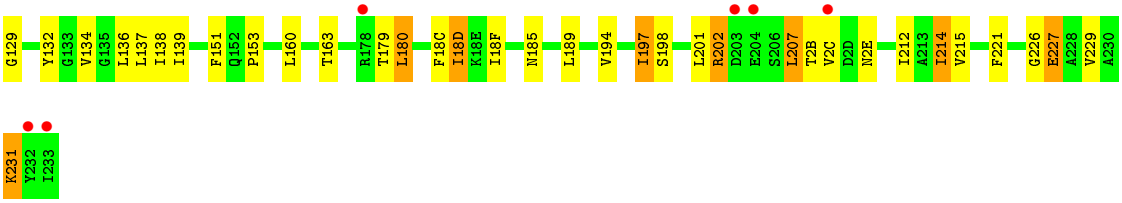




• Molecule 5: Proteasome component PRE5

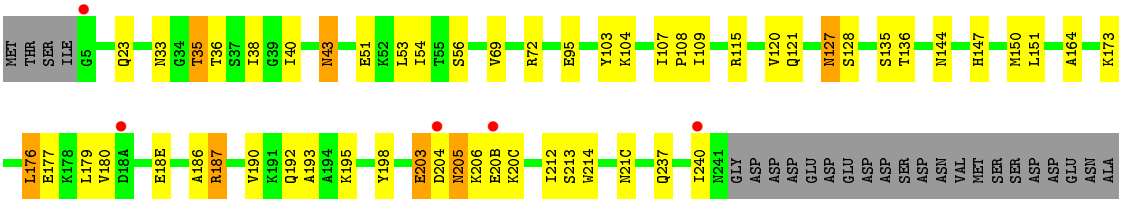
Chain S:

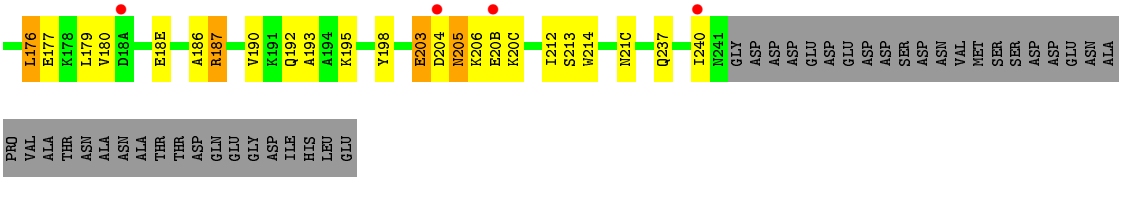




• Molecule 6: Proteasome component C1

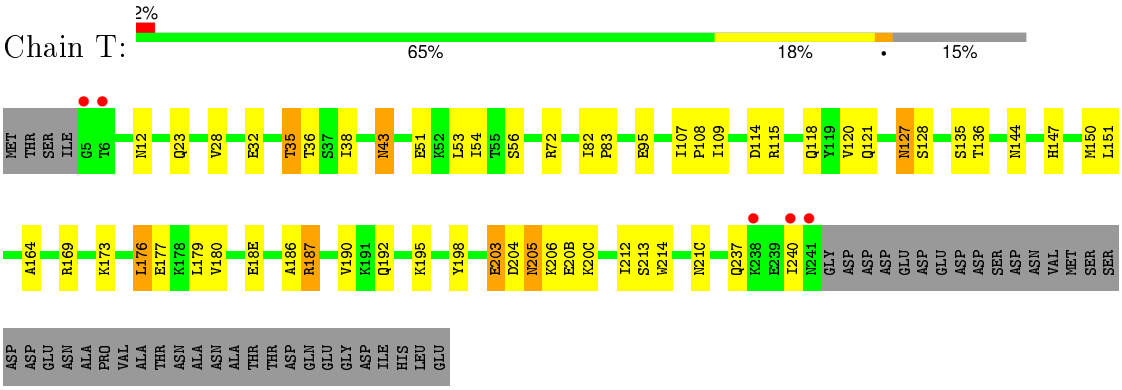
Chain F:





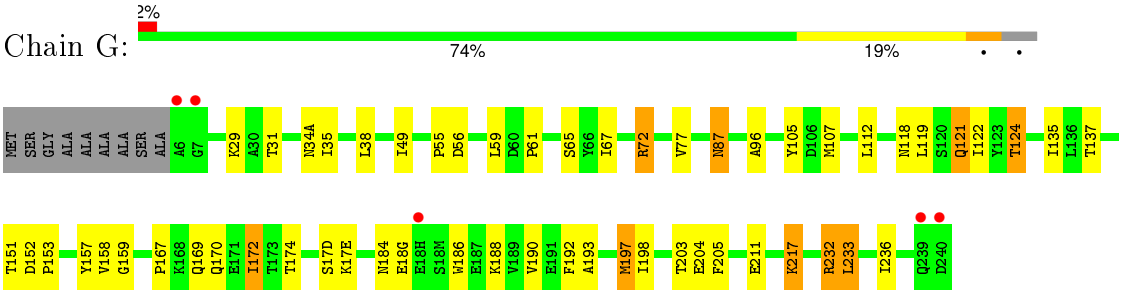
• Molecule 6: Proteasome component C1

Chain T:



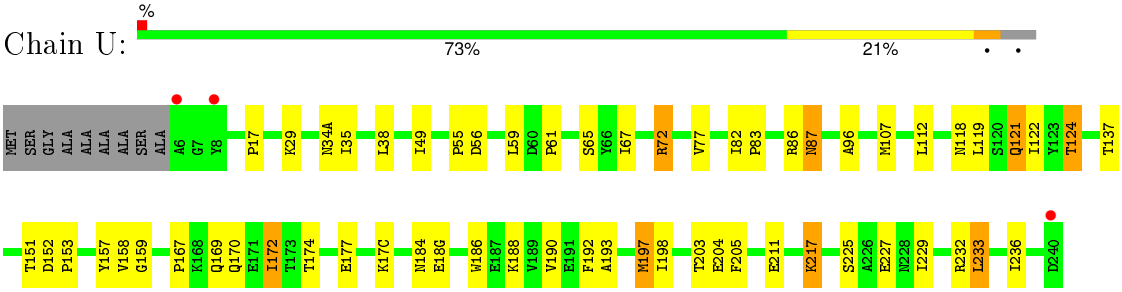
- Molecule 7: Proteasome component C7-alpha

Chain G:



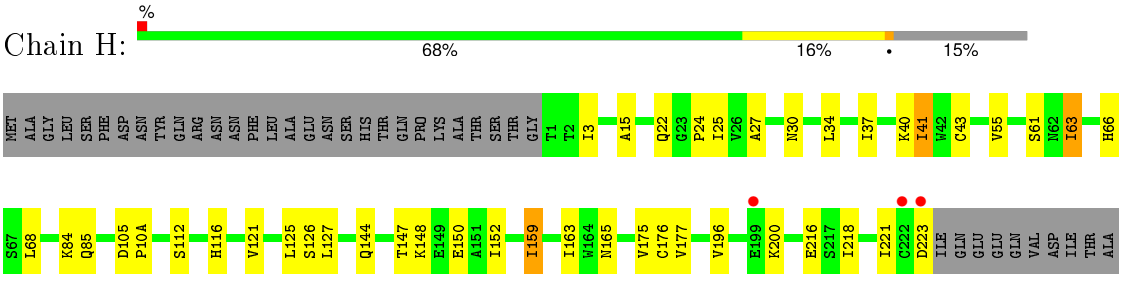
- Molecule 7: Proteasome component C7-alpha

Chain U:



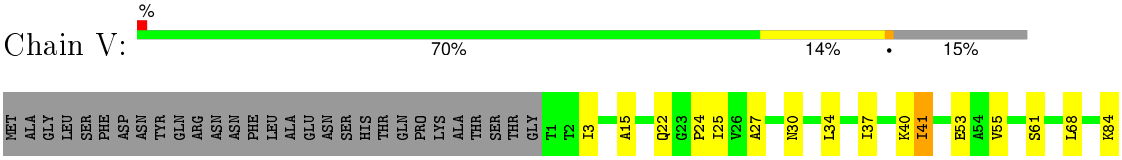
- Molecule 8: Proteasome component PUP1

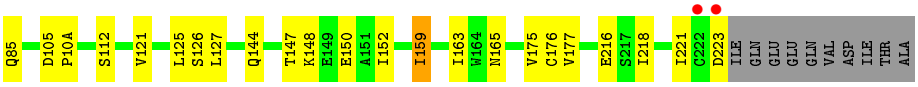
Chain H:



- Molecule 8: Proteasome component PUP1

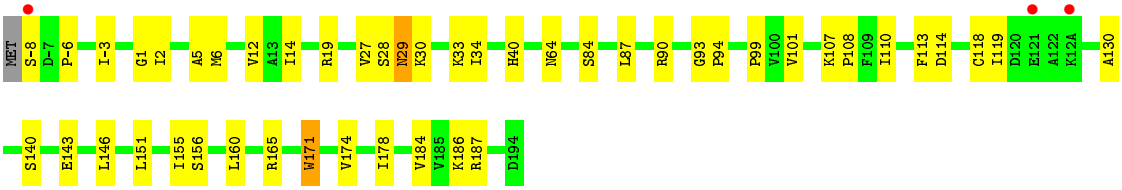
Chain V:





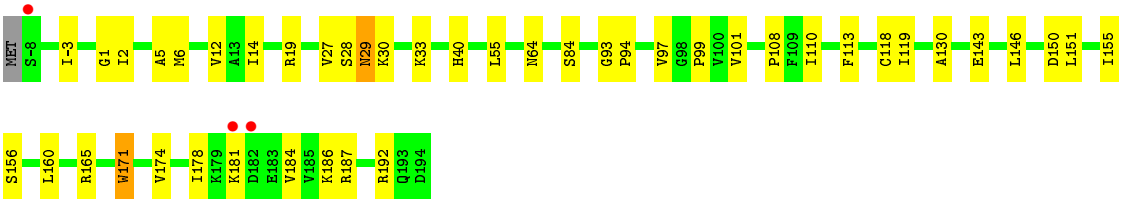
• Molecule 9: Proteasome component PUP3

Chain I:



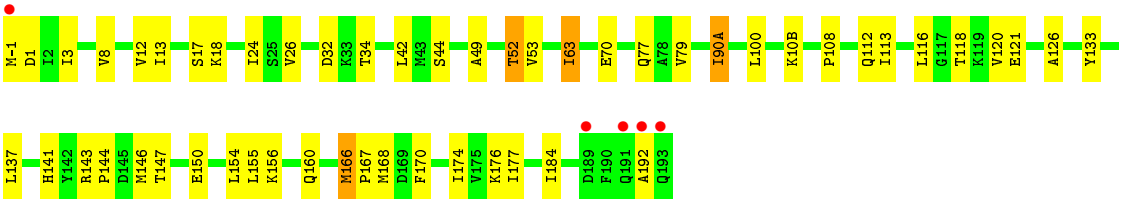
• Molecule 9: Proteasome component PUP3

Chain W:



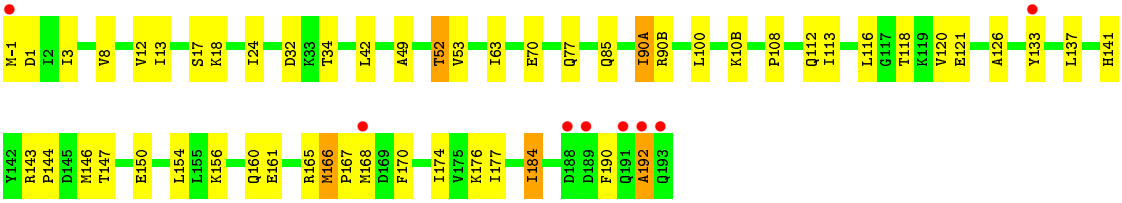
• Molecule 10: Proteasome component C11

Chain J:



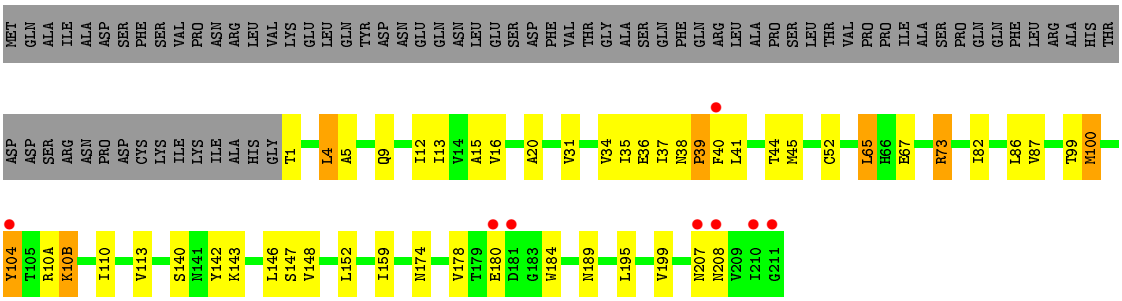
• Molecule 10: Proteasome component C11

Chain X:



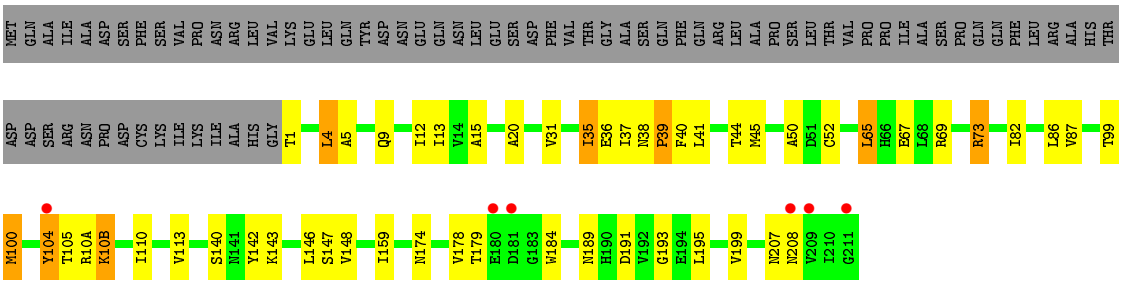
• Molecule 11: Proteasome component PRE2

Chain K:



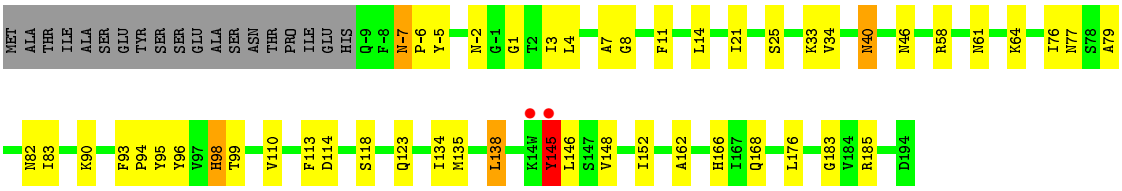
• Molecule 11: Proteasome component PRE2

Chain Y:



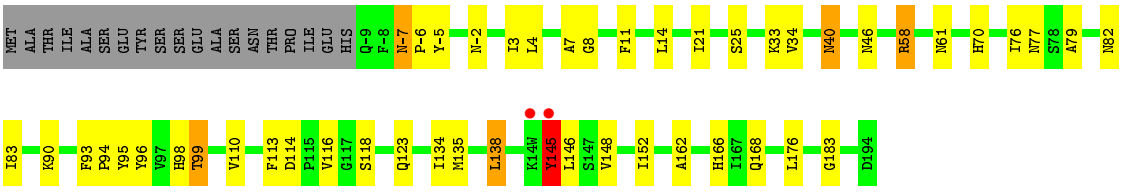
• Molecule 12: Proteasome component C5

Chain L:



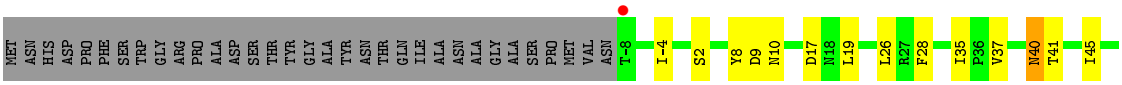
• Molecule 12: Proteasome component C5

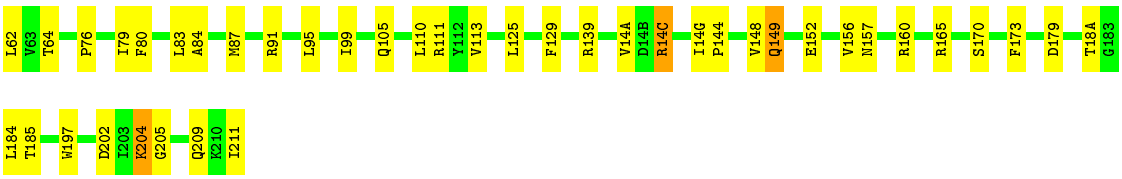
Chain Z:



• Molecule 13: Proteasome component PRE4

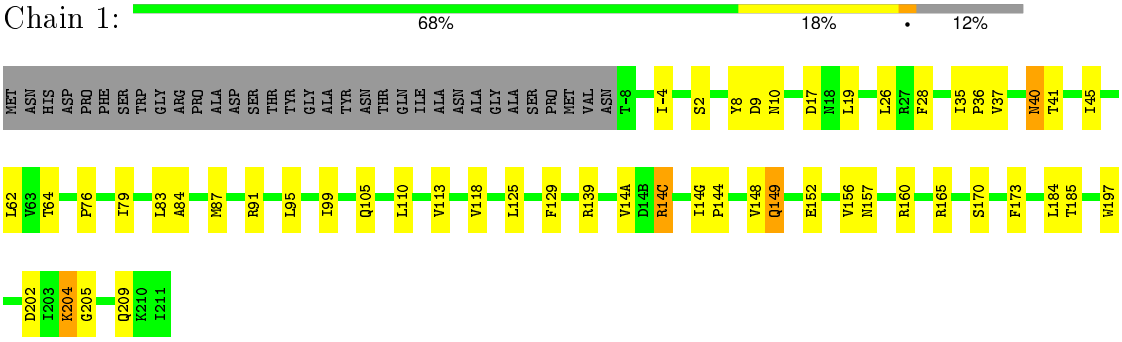
Chain M:





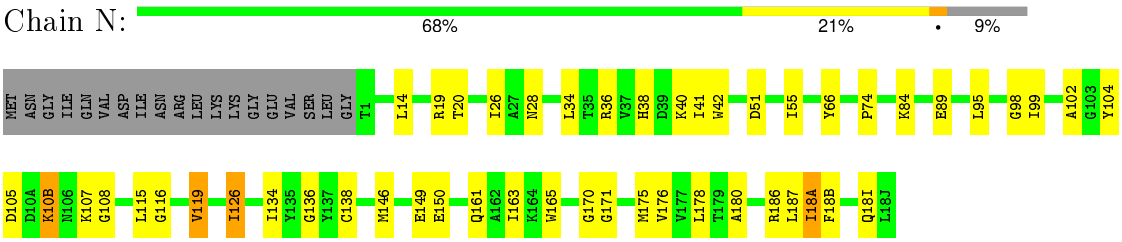
- Molecule 13: Proteasome component PRE4

Chain 1:



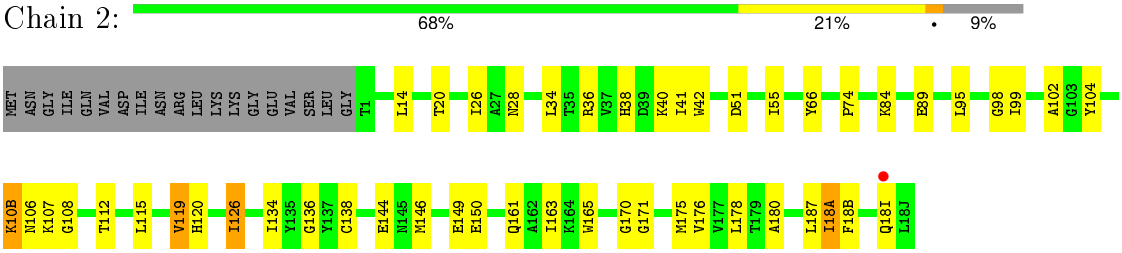
- Molecule 14: Proteasome component PRE3

Chain N:



- Molecule 14: Proteasome component PRE3

Chain 2:



- Molecule 15: TMC-95A mimic ligand 2a

Chain 3:

- Molecule 15: TMC-95A mimic ligand 2a

Chain 4:


?1
Y2
?5

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	136.48Å 301.13Å 145.37Å 90.00° 113.57° 90.00°	Depositor
Resolution (Å)	15.00 – 2.40 49.51 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.5 (15.00-2.40) 99.7 (49.51-2.40)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.95 (at 2.39Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.233 , 0.249 0.220 , 0.220	Depositor DCC
R_{free} test set	20710 reflections (5.00%)	DCC
Wilson B-factor (Å^2)	40.2	Xtriage
Anisotropy	0.786	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 40.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	0 of 415923 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	51006	wwPDB-VP
Average B, all atoms (Å^2)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.28% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: TY5, BOC, ABN, TRO, 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	0.39	0/1952	0.64	0/2642
1	O	0.39	0/1952	0.64	0/2642
2	B	0.38	0/1934	0.63	0/2618
2	P	0.39	0/1934	0.63	0/2618
3	C	0.37	0/1919	0.61	0/2598
3	Q	0.37	0/1919	0.61	0/2598
4	D	0.37	0/1886	0.63	1/2541 (0.0%)
4	R	0.37	0/1886	0.63	0/2541
5	E	0.37	0/1823	0.60	0/2463
5	S	0.37	0/1823	0.61	0/2463
6	F	0.38	0/1936	0.62	0/2614
6	T	0.40	0/1936	0.62	0/2614
7	G	0.43	0/1959	0.63	0/2652
7	U	0.42	0/1959	0.63	0/2652
8	H	0.41	1/1715 (0.1%)	0.67	0/2326
8	V	0.41	0/1715	0.68	0/2326
9	I	0.41	0/1611	0.67	0/2174
9	W	0.41	0/1611	0.68	0/2174
10	J	0.41	0/1613	0.65	0/2173
10	X	0.41	0/1613	0.66	0/2173
11	K	0.41	0/1681	0.67	0/2274
11	Y	0.41	0/1681	0.67	0/2274
12	L	0.42	0/1795	0.68	0/2420
12	Z	0.42	0/1795	0.67	0/2420
13	1	0.42	0/1855	0.68	1/2514 (0.0%)
13	M	0.41	0/1855	0.68	1/2514 (0.0%)
14	2	0.40	0/1541	0.64	0/2087
14	N	0.41	0/1541	0.64	0/2087
15	3	1.25	0/4	0.49	0/4
15	4	1.15	0/4	0.53	0/4
All	All	0.40	1/50448 (0.0%)	0.65	3/68200 (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
1	O	0	1
12	L	0	1
12	Z	0	1
All	All	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	H	43	CYS	CB-SG	-5.11	1.73	1.81

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	1	95	LEU	N-CA-C	-5.74	95.49	111.00
13	M	95	LEU	N-CA-C	-5.60	95.88	111.00
4	D	128	MET	N-CA-C	-5.03	97.43	111.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
12	L	145	TYR	Sidechain
1	O	78	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	36	0
1	O	1915	0	1926	40	0
2	B	1904	0	1901	60	0
2	P	1904	0	1901	64	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	1890	0	1900	73	0
3	Q	1890	0	1900	78	0
4	D	1861	0	1836	40	0
4	R	1861	0	1836	41	0
5	E	1795	0	1797	68	0
5	S	1795	0	1797	63	0
6	F	1896	0	1886	41	0
6	T	1896	0	1886	42	0
7	G	1921	0	1910	48	0
7	U	1921	0	1910	57	0
8	H	1684	0	1688	30	0
8	V	1684	0	1688	27	0
9	I	1581	0	1574	42	0
9	W	1581	0	1574	40	0
10	J	1585	0	1590	62	0
10	X	1585	0	1590	62	0
11	K	1644	0	1595	63	0
11	Y	1644	0	1595	62	0
12	L	1757	0	1711	39	0
12	Z	1757	0	1711	40	0
13	1	1824	0	1832	41	0
13	M	1824	0	1832	42	0
14	2	1512	0	1481	42	0
14	N	1512	0	1481	45	0
15	3	54	0	44	7	0
15	4	54	0	44	7	0
16	K	12	0	13	0	0
16	Y	12	0	13	0	0
17	1	70	0	0	1	0
17	2	60	0	0	1	0
17	A	58	0	0	0	0
17	B	39	0	0	1	0
17	C	43	0	0	1	0
17	D	38	0	0	1	0
17	E	22	0	0	1	0
17	F	48	0	0	2	0
17	G	62	0	0	0	0
17	H	51	0	0	3	0
17	I	65	0	0	2	0
17	J	52	0	0	1	0
17	K	42	0	0	3	0
17	L	57	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	M	71	0	0	2	0
17	N	61	0	0	2	0
17	O	33	0	0	0	0
17	P	30	0	0	2	0
17	Q	26	0	0	2	0
17	R	31	0	0	2	0
17	S	19	0	0	1	0
17	T	40	0	0	2	0
17	U	61	0	0	3	0
17	V	49	0	0	3	0
17	W	61	0	0	1	0
17	X	48	0	0	3	0
17	Y	48	0	0	2	0
17	Z	51	0	0	3	0
All	All	51006	0	49368	1238	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 12.

The worst 5 of 1238 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)
7:U:96:ALA:HA	7:U:107:MET:HE2	1.31	1.12
11:Y:10(B):LYS:H	11:Y:10(B):LYS:HD2	1.13	1.09
11:K:10(B):LYS:H	11:K:10(B):LYS:HD2	1.11	1.08
2:P:202:THR:HG22	2:P:204:SER:H	1.21	1.06
7:G:96:ALA:HA	7:G:107:MET:HE2	1.33	1.05

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%)	236 (95%)	10 (4%)	2 (1%)	24	35
1	O	248/250 (99%)	236 (95%)	10 (4%)	2 (1%)	24	35
2	B	242/258 (94%)	222 (92%)	16 (7%)	4 (2%)	11	14
2	P	242/258 (94%)	224 (93%)	14 (6%)	4 (2%)	11	14
3	C	239/254 (94%)	224 (94%)	9 (4%)	6 (2%)	7	7
3	Q	239/254 (94%)	222 (93%)	11 (5%)	6 (2%)	7	7
4	D	240/260 (92%)	228 (95%)	8 (3%)	4 (2%)	11	14
4	R	240/260 (92%)	228 (95%)	8 (3%)	4 (2%)	11	14
5	E	231/234 (99%)	213 (92%)	15 (6%)	3 (1%)	15	21
5	S	231/234 (99%)	213 (92%)	15 (6%)	3 (1%)	15	21
6	F	242/288 (84%)	234 (97%)	7 (3%)	1 (0%)	39	56
6	T	242/288 (84%)	233 (96%)	8 (3%)	1 (0%)	39	56
7	G	241/252 (96%)	232 (96%)	9 (4%)	0	100	100
7	U	241/252 (96%)	232 (96%)	9 (4%)	0	100	100
8	H	220/261 (84%)	209 (95%)	11 (5%)	0	100	100
8	V	220/261 (84%)	210 (96%)	10 (4%)	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%)	187 (95%)	6 (3%)	3 (2%)	13	17
10	X	196/198 (99%)	187 (95%)	6 (3%)	3 (2%)	13	17
11	K	210/287 (73%)	204 (97%)	5 (2%)	1 (0%)	34	48
11	Y	210/287 (73%)	204 (97%)	5 (2%)	1 (0%)	34	48
12	L	220/241 (91%)	214 (97%)	6 (3%)	0	100	100
12	Z	220/241 (91%)	214 (97%)	6 (3%)	0	100	100
13	1	231/266 (87%)	220 (95%)	10 (4%)	1 (0%)	39	56
13	M	231/266 (87%)	220 (95%)	10 (4%)	1 (0%)	39	56
14	2	194/215 (90%)	184 (95%)	10 (5%)	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
All	All	6314/6948 (91%)	6009 (95%)	255 (4%)	50 (1%)	24	35

5 of 50 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	21(C)	ASP
3	C	58	LEU
4	D	12(G)	GLU
11	K	39	PRO
2	P	21(C)	ASP

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	209/209 (100%)	203 (97%)	6 (3%)	50	71
1	O	209/209 (100%)	204 (98%)	5 (2%)	57	76
2	B	203/216 (94%)	193 (95%)	10 (5%)	31	48
2	P	203/216 (94%)	193 (95%)	10 (5%)	31	48
3	C	213/226 (94%)	200 (94%)	13 (6%)	23	36
3	Q	213/226 (94%)	200 (94%)	13 (6%)	23	36
4	D	198/215 (92%)	186 (94%)	12 (6%)	23	36
4	R	198/215 (92%)	187 (94%)	11 (6%)	26	41
5	E	192/193 (100%)	173 (90%)	19 (10%)	10	14
5	S	192/193 (100%)	174 (91%)	18 (9%)	11	16
6	F	201/239 (84%)	185 (92%)	16 (8%)	15	23
6	T	201/239 (84%)	184 (92%)	17 (8%)	13	20
7	G	207/210 (99%)	194 (94%)	13 (6%)	22	35
7	U	207/210 (99%)	195 (94%)	12 (6%)	25	39
8	H	181/214 (85%)	171 (94%)	10 (6%)	27	42
8	V	181/214 (85%)	172 (95%)	9 (5%)	30	48
9	I	172/173 (99%)	168 (98%)	4 (2%)	58	78
9	W	172/173 (99%)	168 (98%)	4 (2%)	58	78
10	J	175/175 (100%)	167 (95%)	8 (5%)	33	51
10	X	175/175 (100%)	166 (95%)	9 (5%)	29	46

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
11	K	169/235 (72%)	158 (94%)	11 (6%)	21 33
11	Y	169/235 (72%)	158 (94%)	11 (6%)	21 33
12	L	185/201 (92%)	174 (94%)	11 (6%)	24 38
12	Z	185/201 (92%)	174 (94%)	11 (6%)	24 38
13	1	199/224 (89%)	192 (96%)	7 (4%)	43 64
13	M	199/224 (89%)	192 (96%)	7 (4%)	43 64
14	2	162/178 (91%)	154 (95%)	8 (5%)	31 48
14	N	162/178 (91%)	155 (96%)	7 (4%)	35 55
All	All	5332/5816 (92%)	5040 (94%)	292 (6%)	27 42

5 of 292 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
12	L	145	TYR
3	Q	14	ILE
12	Z	25	SER
13	M	91	ARG
1	O	64	LEU

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

Mol	Chain	Res	Type
12	L	166	HIS
2	P	218	ASN
12	Z	82	ASN
13	M	89	GLN
14	N	161	GLN

5.3.3 RNA (i)

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	1.66	3 (15%)	22,25,27	1.22	3 (13%)
15	TRO	3	4	15	13,16,17	3.04	5 (38%)	11,22,24	2.15	2 (18%)
15	TY5	4	2	15	19,20,21	1.65	3 (15%)	22,25,27	1.19	3 (13%)
15	TRO	4	4	15	13,16,17	3.03	5 (38%)	11,22,24	2.12	2 (18%)

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	-	0/9/11/13	0/2/2/2
15	TRO	3	4	15	-	0/2/6/8	0/2/2/2
15	TY5	4	2	15	-	0/9/11/13	0/2/2/2
15	TRO	4	4	15	-	0/2/6/8	0/2/2/2

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	4	2	TY5	CD1-CG	2.02	1.43	1.38
15	4	4	TRO	CZ3-CH2	2.06	1.43	1.38
15	3	2	TY5	CE2-CD2	2.10	1.42	1.38
15	3	2	TY5	CD1-CG	2.12	1.43	1.38
15	4	2	TY5	CE2-CD2	2.14	1.42	1.38

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	3	4	TRO	CB-CG-CD1	-5.12	112.84	124.01
15	4	4	TRO	CB-CG-CD1	-5.08	112.94	124.01
15	3	4	TRO	O-C-CA	-2.99	117.71	125.49
15	4	4	TRO	O-C-CA	-2.99	117.71	125.49
15	3	2	TY5	O-C-CA	-2.58	118.77	125.49

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 carbohydrates 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	K	212	-	11,12,12	1.78	2 (18%)	14,16,16	2.44	4 (28%)
16	MES	Y	212	-	11,12,12	1.78	1 (9%)	14,16,16	2.51	4 (28%)

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

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	K	212	MES	O1-C6	-4.30	1.24	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	Y	212	MES	O1-C6	-4.29	1.24	1.42
16	K	212	MES	O2S-S	2.06	1.51	1.45

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	Y	212	MES	O2S-S-C8	-6.46	101.39	106.91
16	K	212	MES	O2S-S-C8	-5.73	102.01	106.91
16	Y	212	MES	C7-N4-C3	3.15	119.34	111.27
16	K	212	MES	O3S-S-O1S	3.21	119.07	111.61
16	Y	212	MES	O3S-S-O1S	3.29	119.27	111.61

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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%)	-0.29	4 (1%)	74	74	35, 49, 79, 105	0
1	O	250/250 (100%)	-0.21	6 (2%)	62	61	37, 51, 81, 104	0
2	B	244/258 (94%)	-0.13	6 (2%)	61	60	36, 53, 91, 117	0
2	P	244/258 (94%)	-0.03	11 (4%)	37	38	37, 54, 93, 117	0
3	C	241/254 (94%)	-0.02	11 (4%)	36	37	39, 56, 110, 125	0
3	Q	241/254 (94%)	0.29	30 (12%)	5	5	39, 59, 111, 125	0
4	D	242/260 (93%)	-0.07	8 (3%)	50	50	39, 57, 92, 123	0
4	R	242/260 (93%)	-0.07	9 (3%)	45	46	40, 58, 91, 123	0
5	E	233/234 (99%)	-0.04	8 (3%)	49	49	42, 59, 86, 111	0
5	S	233/234 (99%)	-0.02	10 (4%)	39	40	42, 60, 87, 111	0
6	F	244/288 (84%)	-0.21	5 (2%)	68	68	36, 52, 90, 106	0
6	T	244/288 (84%)	-0.18	5 (2%)	68	68	36, 53, 91, 107	0
7	G	243/252 (96%)	-0.31	5 (2%)	67	66	34, 48, 76, 115	0
7	U	243/252 (96%)	-0.35	3 (1%)	81	81	35, 48, 75, 115	0
8	H	222/261 (85%)	-0.32	3 (1%)	78	77	35, 47, 69, 97	0
8	V	222/261 (85%)	-0.36	2 (0%)	85	85	35, 48, 69, 97	0
9	I	204/205 (99%)	-0.30	3 (1%)	76	75	34, 47, 67, 82	0
9	W	204/205 (99%)	-0.20	3 (1%)	76	75	36, 48, 68, 82	0
10	J	198/198 (100%)	-0.27	5 (2%)	61	60	34, 48, 66, 124	0
10	X	198/198 (100%)	-0.35	8 (4%)	42	43	36, 49, 66, 125	0
11	K	212/287 (73%)	-0.20	8 (3%)	44	45	33, 48, 75, 85	0
11	Y	212/287 (73%)	-0.17	6 (2%)	56	55	35, 49, 76, 86	0
12	L	222/241 (92%)	-0.36	2 (0%)	85	85	34, 47, 70, 96	0
12	Z	222/241 (92%)	-0.35	2 (0%)	85	85	35, 47, 69, 96	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	1	233/266 (87%)	-0.53	0 100 100	34, 46, 61, 68	0
13	M	233/266 (87%)	-0.44	1 (0%) 93 93	32, 46, 62, 66	0
14	2	196/215 (91%)	-0.38	1 (0%) 91 91	33, 44, 67, 80	0
14	N	196/215 (91%)	-0.48	0 100 100	34, 44, 67, 80	0
15	3	1/5 (20%)	-0.16	0 100 100	52, 52, 52, 52	0
15	4	1/5 (20%)	-0.19	0 100 100	55, 55, 55, 55	0
All	All	6370/6948 (91%)	-0.22	165 (2%) 59 58	32, 50, 83, 125	0

The worst 5 of 165 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	D	12(D)	ALA	13.8
4	D	12(E)	SER	11.1
4	R	12(F)	GLY	11.1
10	J	192	ALA	9.3
3	Q	56	LEU	9.0

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å^2)	Q<0.9
15	TRO	3	4	15/16	0.93	0.16	-	53,62,64,65	0
15	TY5	3	2	19/20	0.94	0.22	-	57,61,70,70	0
15	TY5	4	2	19/20	0.93	0.17	-	58,60,70,70	0
15	TRO	4	4	15/16	0.89	0.19	-	56,63,64,65	0

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å^2)	Q<0.9
16	MES	K	212	12/12	0.95	0.18	3.11	71,75,78,78	0
16	MES	Y	212	12/12	0.93	0.15	0.90	74,77,79,79	0

6.5 Other polymers

There are no such residues in this entry.