



wwPDB X-ray Structure Validation Summary Report ⓘ

May 24, 2016 – 03:53 PM EDT

PDB ID : 4ZZG
Title : Yeast 20S proteasome in complex with Blm-pep activator
Authors : Witkowska, J.; Grudnik, P.; Golik, P.; Dubin, G.; Jankowska, E.
Deposited on : 2015-05-22
Resolution : 3.00 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 ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20027674
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) : rb-20027674

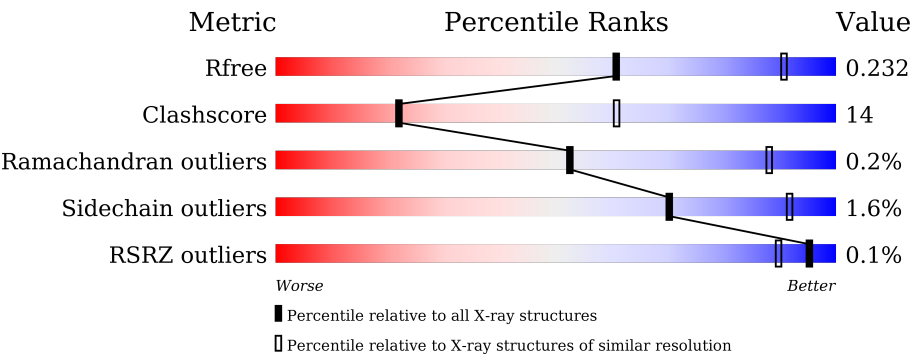
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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.













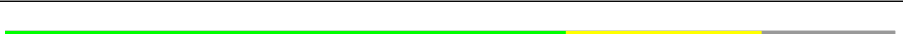



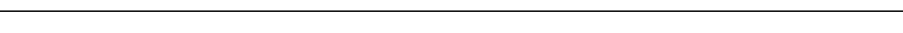
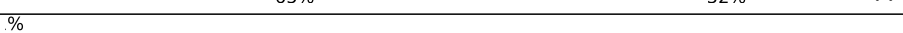








Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	252	<div><div>68%</div><div>26%</div><div>••</div></div>
1	O	252	<div><div>67%</div><div>28%</div><div>••</div></div>
2	B	250	<div><div>71%</div><div>28%</div><div>•</div></div>
2	P	250	<div><div>74%</div><div>26%</div><div></div></div>
3	C	258	<div><div>64%</div><div>29%</div><div>7%</div></div>
3	Q	258	<div><div>68%</div><div>26%</div><div>6%</div></div>

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

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
18	EDO	2	304	-	-	-	X
18	EDO	C	302	-	-	-	X
18	EDO	G	301	-	-	-	X
18	EDO	L	302	-	-	-	X
18	EDO	O	302	-	-	-	X
18	EDO	O	303	-	-	-	X
18	EDO	U	301	-	-	-	X
18	EDO	W	303	-	-	-	X
18	EDO	Y	202	-	-	-	X
19	GOL	K	203	-	-	-	X
19	GOL	L	301	-	-	-	X
19	GOL	Q	301	-	-	-	X
19	GOL	V	203	-	-	-	X

2 Entry composition

There are 20 unique types of molecules in this entry. The entry contains 49522 atoms, of which 104 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 subunit alpha type-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	241	Total	C	N	O	S	0	0	0
			1907	1214	320	365	8			
1	O	242	Total	C	N	O	S	0	0	0
			1901	1210	319	364	8			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	250	Total	C	N	O	S	0	0	0
			1907	1213	313	377	4			
2	P	250	Total	C	N	O	S	0	0	0
			1915	1219	315	377	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	241	Total	C	N	O	S	0	0	0
			1875	1183	314	375	3			
3	Q	242	Total	C	N	O	S	0	0	0
			1866	1178	311	374	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	241	Total	C	N	O	S	0	0	0
			1850	1153	324	369	4			
4	R	241	Total	C	N	O	S	0	0	0
			1855	1158	325	368	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	236	Total	C	N	O	S	0	0	0
			1815	1140	302	366	7			
5	S	236	Total	C	N	O	S	0	0	0
			1818	1139	305	367	7			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	232	Total	C	N	O	S	0	0	0
			1772	1114	305	349	4			
6	T	232	Total	C	N	O	S	0	0	0
			1776	1115	309	348	4			

- Molecule 7 is a protein called Probable proteasome subunit alpha type-7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	244	Total	C	N	O	S	0	0	0
			1880	1194	327	355	4			
7	U	244	Total	C	N	O	S	0	0	0
			1884	1197	328	355	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	196	Total	C	N	O	S	0	0	0
			1512	955	250	300	7			
8	V	196	Total	C	N	O	S	0	0	0
			1512	955	250	300	7			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	222	Total	C	N	O	S	0	0	0
			1684	1061	293	323	7			
9	W	222	Total	C	N	O	S	0	0	0
			1684	1061	293	323	7			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	204	Total	C	N	O	S	0	0	0
			1581	1010	258	305	8			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	X	204	Total	C	N	O	S	0	0	0
			1577	1007	257	305	8			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	196	Total	C	N	O	S	0	0	0
			1563	994	265	298	6			
11	Y	196	Total	C	N	O	S	0	0	0
			1566	995	265	300	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	212	Total	C	N	O	S	0	0	0
			1640	1042	279	312	7			
12	Z	212	Total	C	N	O	S	0	0	0
			1644	1045	280	312	7			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	222	Total	C	N	O	S	0	0	0
			1745	1106	300	335	4			
13	1	222	Total	C	N	O	S	0	0	0
			1753	1112	302	335	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	N	232	Total	C	N	O	S	0	0	0
			1817	1150	311	349	7			
14	2	233	Total	C	N	O	S	0	0	0
			1824	1154	312	351	7			

- Molecule 15 is a protein called Synthetic peptide (polymer).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	3	6	Total	C	N	O	0	0	0
			52	33	9	10			
15	4	6	Total	C	N	O	0	0	0
			52	33	9	10			

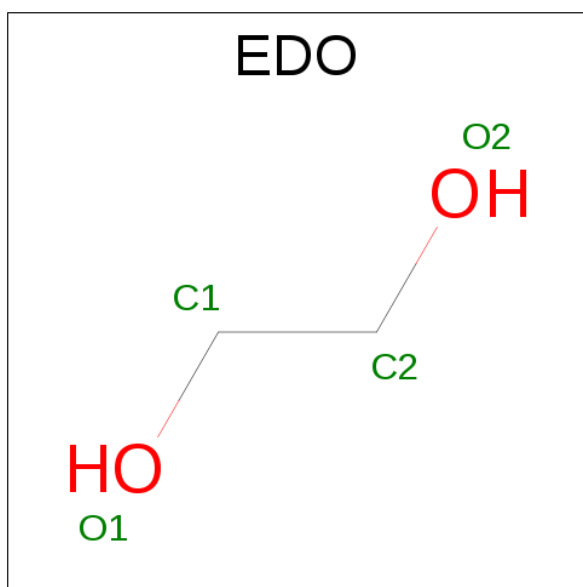
- Molecule 16 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	2	3	Total 3	Cl 3	0	0
16	K	2	Total 2	Cl 2	0	0
16	V	2	Total 2	Cl 2	0	0
16	A	1	Total 1	Cl 1	0	0
16	N	1	Total 1	Cl 1	0	0
16	O	1	Total 1	Cl 1	0	0
16	R	1	Total 1	Cl 1	0	0
16	S	1	Total 1	Cl 1	0	0

- Molecule 17 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	J	1	Total 1	Mg 1	0	0
17	Q	1	Total 1	Mg 1	0	0
17	D	1	Total 1	Mg 1	0	0
17	H	1	Total 1	Mg 1	0	0
17	I	1	Total 1	Mg 1	0	0
17	C	1	Total 1	Mg 1	0	0
17	N	2	Total 2	Mg 2	0	0

- Molecule 18 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



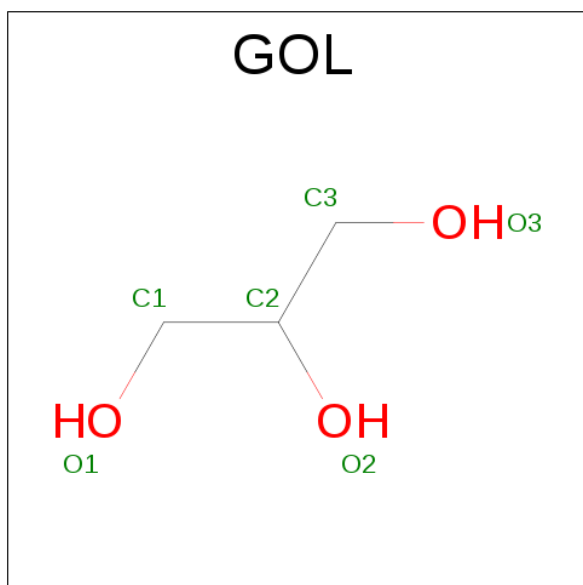
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
18	C	1	Total	C	H	O	0	0
			10	2	6	2		
18	F	1	Total	C	H	O	0	0
			10	2	6	2		
18	G	1	Total	C	H	O	0	0
			10	2	6	2		
18	I	1	Total	C	H	O	0	0
			10	2	6	2		
18	L	1	Total	C	H	O	0	0
			10	2	6	2		
18	M	1	Total	C	H	O	0	0
			10	2	6	2		
18	O	1	Total	C	H	O	0	0
			10	2	6	2		
18	O	1	Total	C	H	O	0	0
			10	2	6	2		
18	U	1	Total	C	H	O	0	0
			10	2	6	2		
18	W	1	Total	C	H	O	0	0
			10	2	6	2		
18	W	1	Total	C	H	O	0	0
			10	2	6	2		
18	W	1	Total	C	H	O	0	0
			10	2	6	2		
18	Y	1	Total	C	H	O	0	0
			10	2	6	2		
18	Y	1	Total	C	H	O	0	0
			10	2	6	2		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
18	1	1	Total	C	H	O	0	0
			10	2	6	2		
18	2	1	Total	C	H	O	0	0
			10	2	6	2		

- Molecule 19 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
19	K	1	Total	C	O		0	0
			6	3	3			
19	L	1	Total	C	O		0	0
			6	3	3			
19	M	1	Total	C	H	O	0	0
			14	3	8	3		
19	Q	1	Total	C	O		0	0
			6	3	3			
19	V	1	Total	C	O		0	0
			6	3	3			
19	Z	1	Total	C	O		0	0
			6	3	3			
19	Z	1	Total	C	O		0	0
			6	3	3			

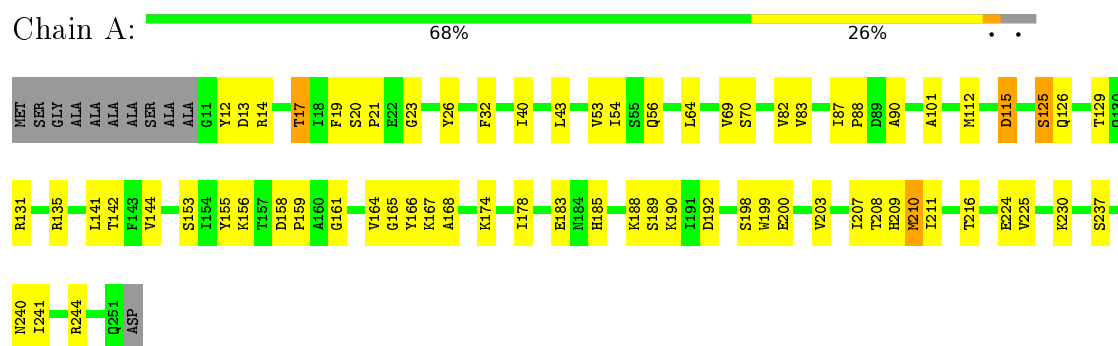
- Molecule 20 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
20	A	2	Total O 2 2	0	0
20	C	2	Total O 2 2	0	0
20	D	1	Total O 1 1	0	0
20	G	2	Total O 2 2	0	0
20	H	8	Total O 8 8	0	0
20	I	2	Total O 2 2	0	0
20	J	1	Total O 1 1	0	0
20	L	1	Total O 1 1	0	0
20	M	4	Total O 4 4	0	0
20	N	4	Total O 4 4	0	0
20	O	4	Total O 4 4	0	0
20	U	2	Total O 2 2	0	0
20	V	4	Total O 4 4	0	0
20	W	3	Total O 3 3	0	0
20	X	2	Total O 2 2	0	0
20	Z	6	Total O 6 6	0	0
20	1	9	Total O 9 9	0	0
20	2	8	Total O 8 8	0	0

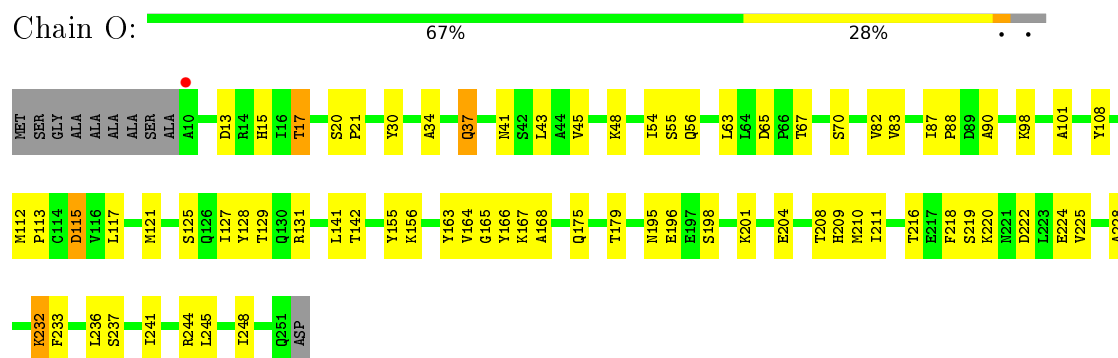
3 Residue-property plots

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.

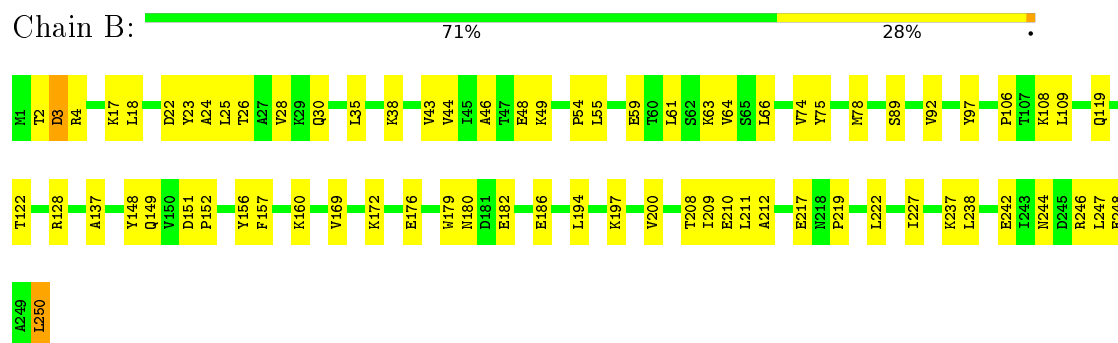
- Molecule 1: Proteasome subunit alpha type-1



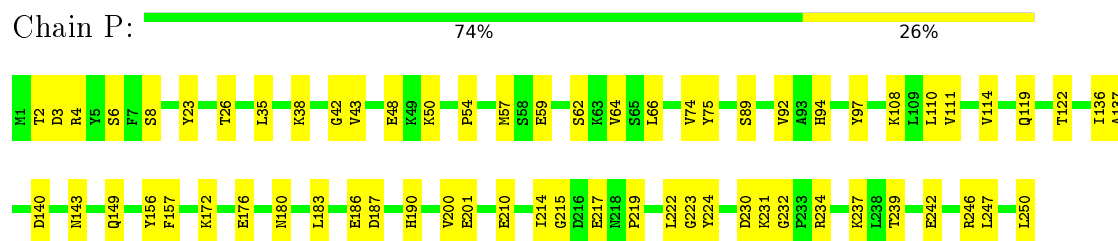
- Molecule 1: Proteasome subunit alpha type-1



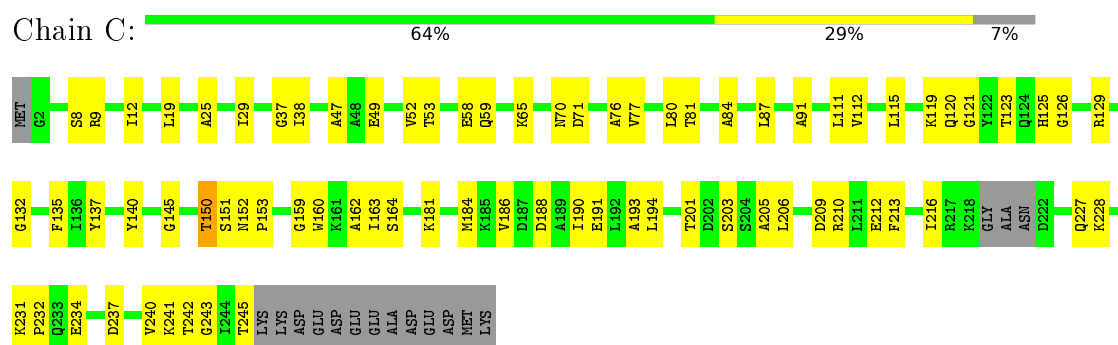
- Molecule 2: Proteasome subunit alpha type-2



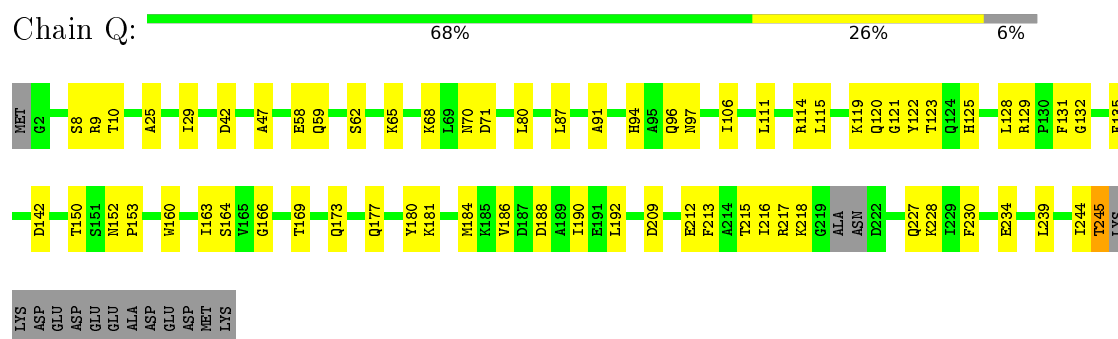
- Molecule 2: Proteasome subunit alpha type-2



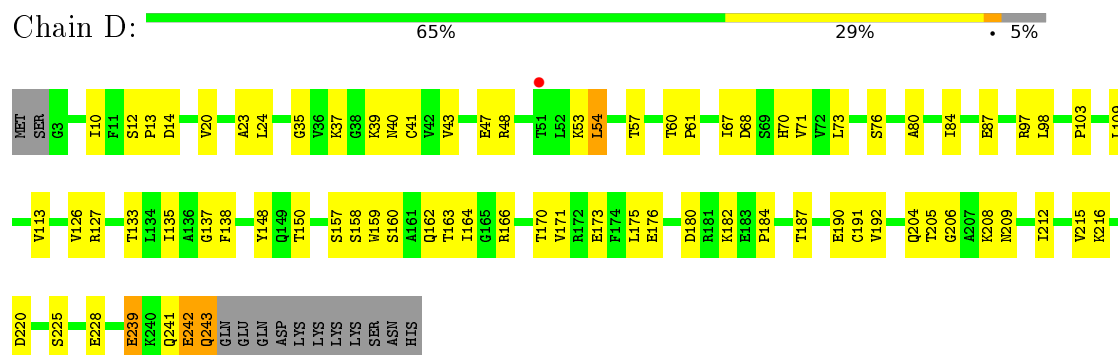
- Molecule 3: Proteasome subunit alpha type-3



- Molecule 3: Proteasome subunit alpha type-3

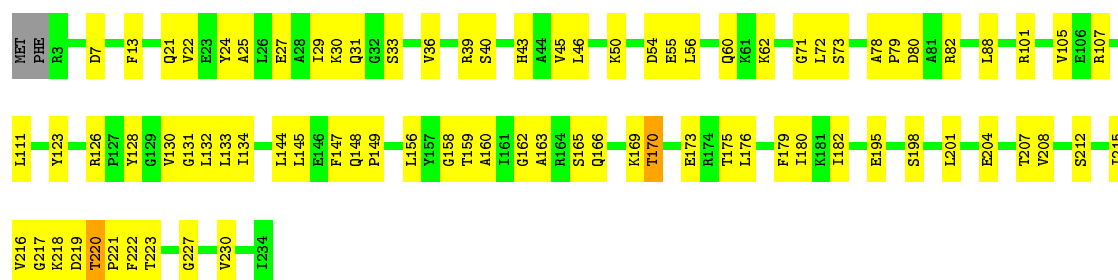


- Molecule 4: Proteasome subunit alpha type-4



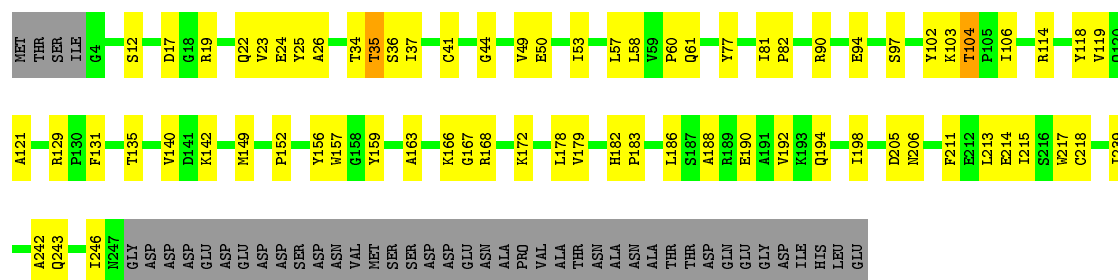
- Molecule 4: Proteasome subunit alpha type-4





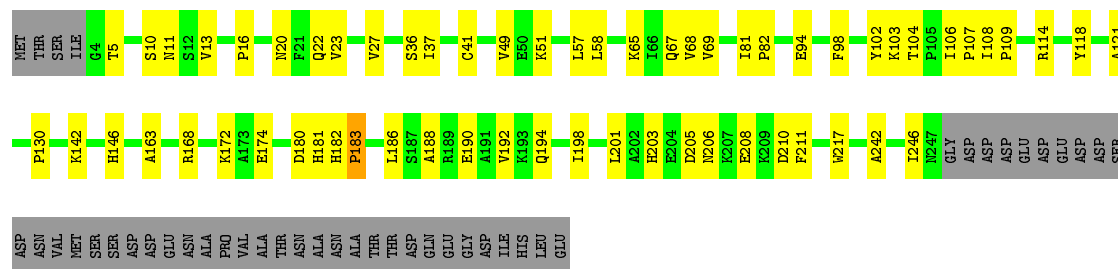
- Molecule 7: Probable proteasome subunit alpha type-7

Chain G: 60% 24% 15%



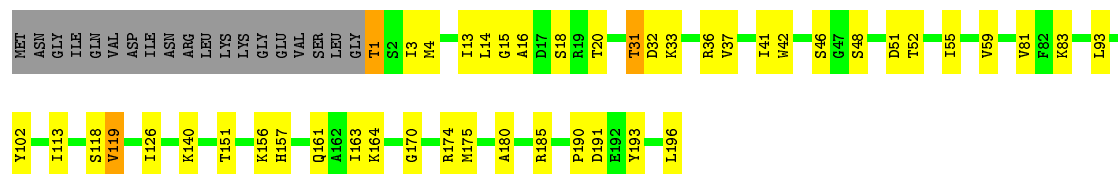
- Molecule 7: Probable proteasome subunit alpha type-7

Chain U: 64% 21% 15%



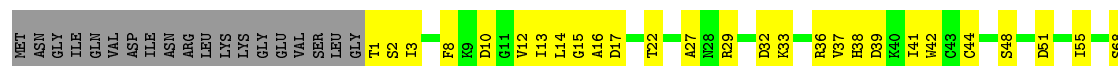
- Molecule 8: Proteasome subunit beta type-1

Chain H: 70% 20% 9%



- Molecule 8: Proteasome subunit beta type-1

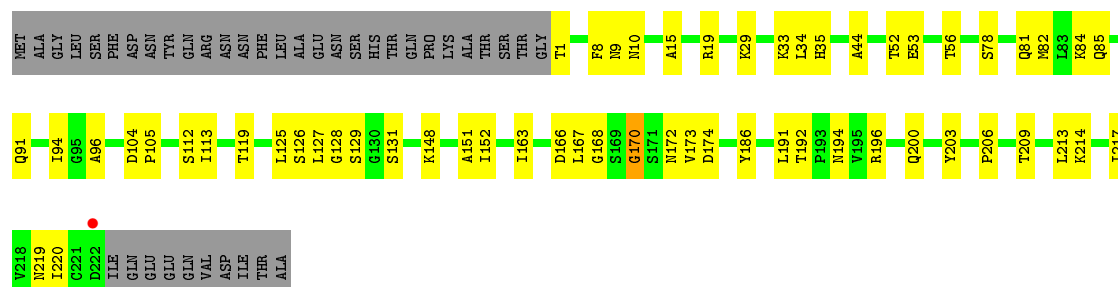
Chain V: 65% 26% 9%





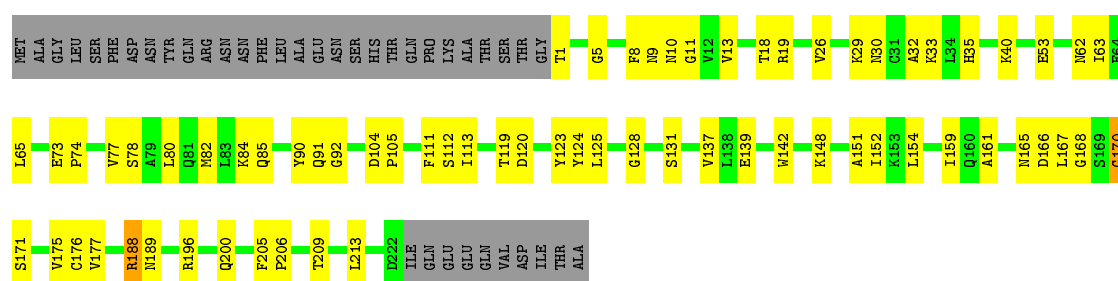
• Molecule 9: Proteasome subunit beta type-2

Chain I: 63% 22% 15%



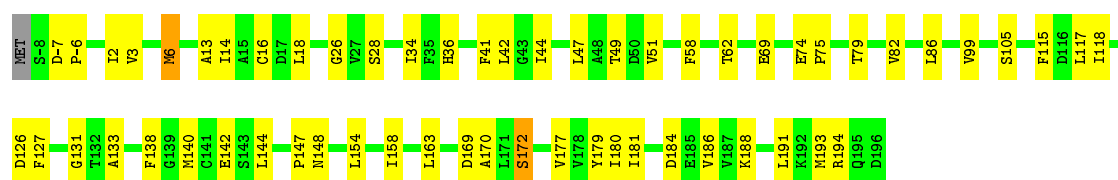
• Molecule 9: Proteasome subunit beta type-2

Chain W: 59% 26% 15%



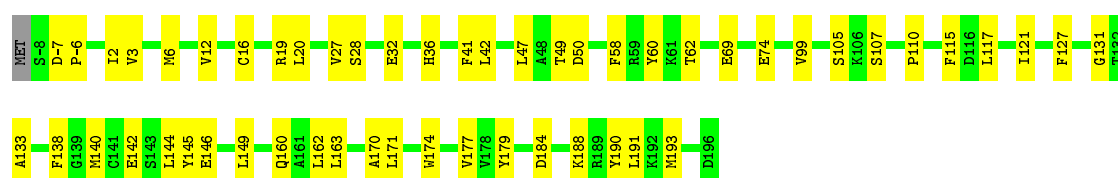
• Molecule 10: Proteasome subunit beta type-3

Chain J: 71% 27%

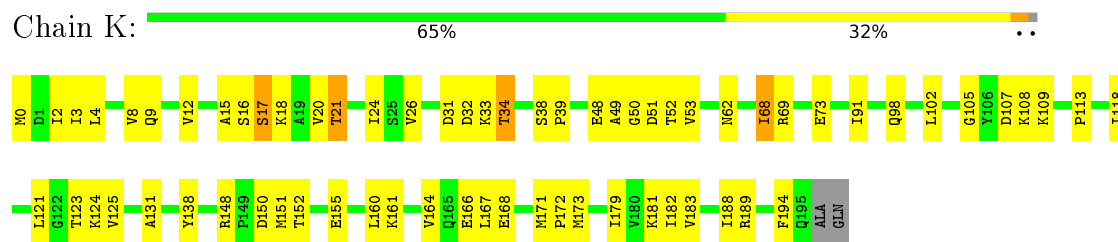


• Molecule 10: Proteasome subunit beta type-3

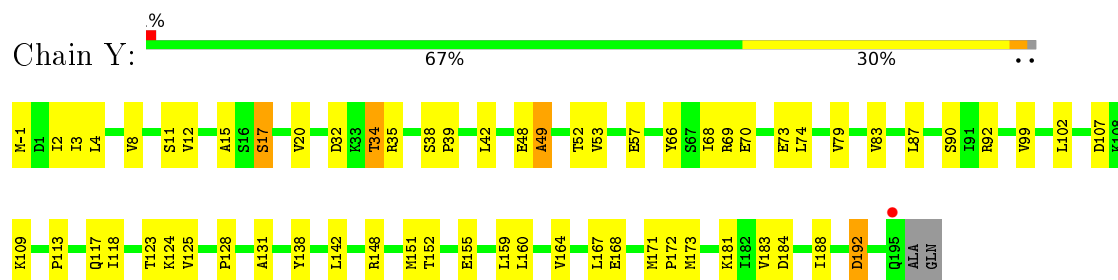
Chain X: 74% 26%



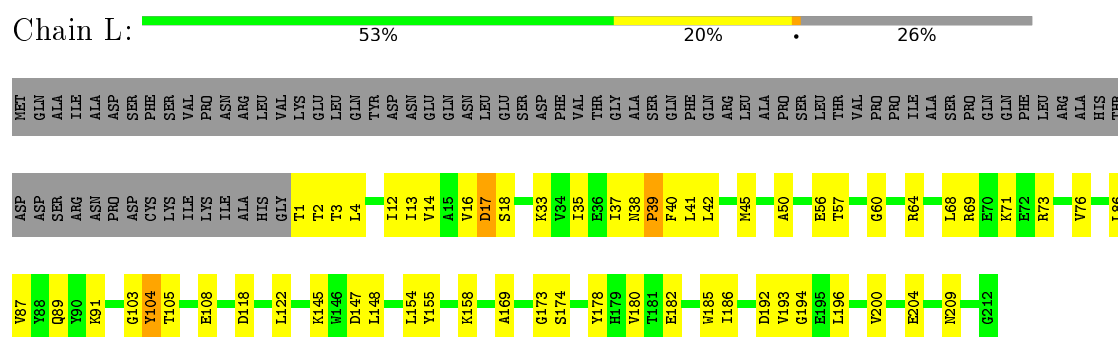
• Molecule 11: Proteasome subunit beta type-4



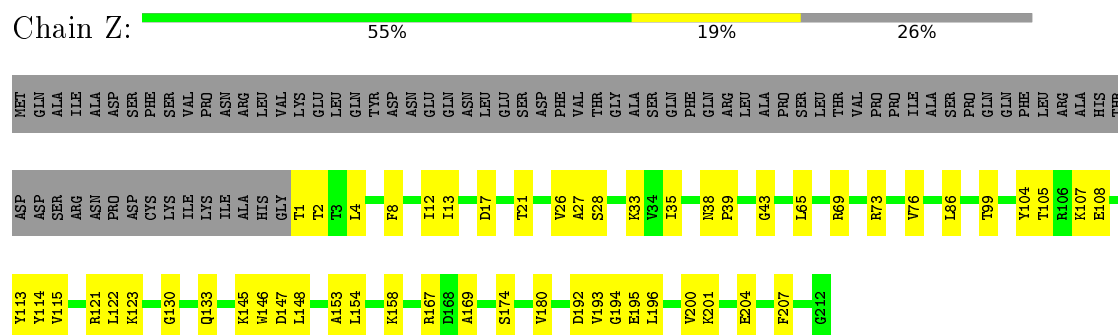
• Molecule 11: Proteasome subunit beta type-4



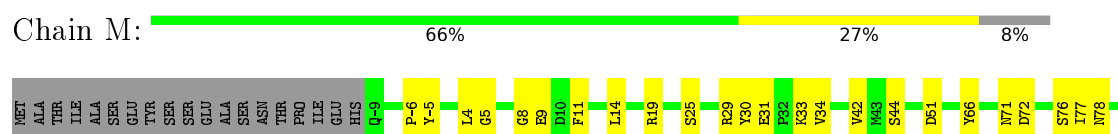
• Molecule 12: Proteasome subunit beta type-5

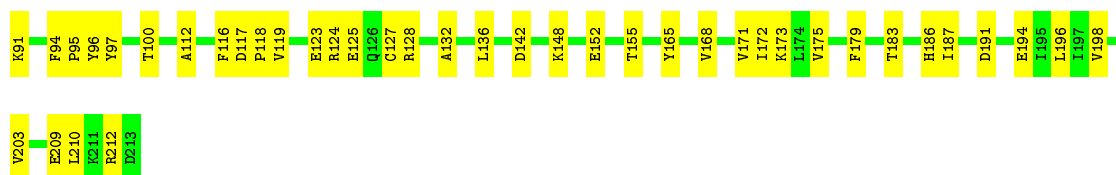


• Molecule 12: Proteasome subunit beta type-5



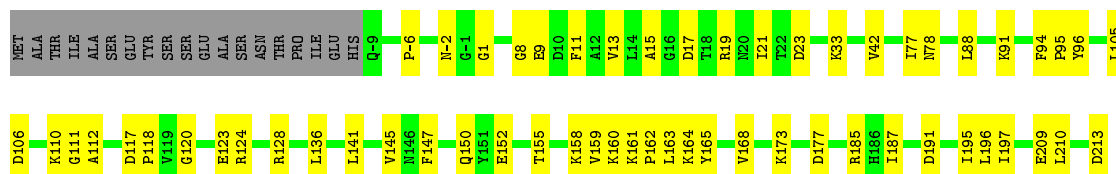
• Molecule 13: Proteasome subunit beta type-6





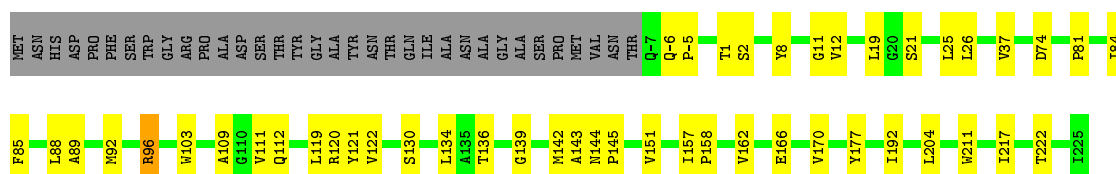
- Molecule 13: Proteasome subunit beta type-6

Chain 1: 68% 24% 8%



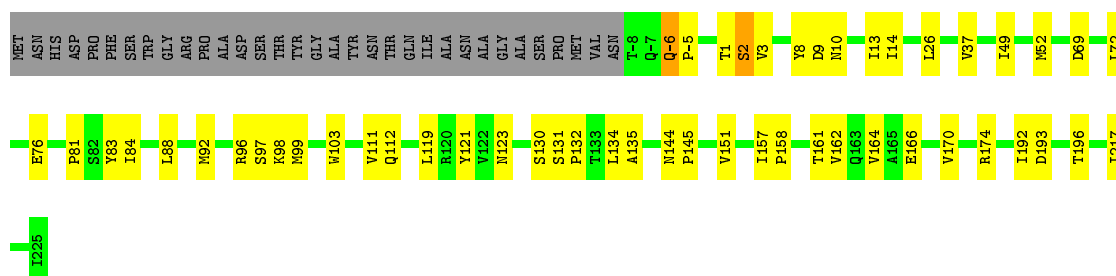
- Molecule 14: Proteasome subunit beta type-7

Chain N: 69% 18% 13%



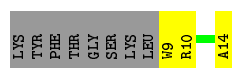
- Molecule 14: Proteasome subunit beta type-7

Chain 2: 68% 19% 12%



- Molecule 15: Synthetic peptide (polymer)

Chain 3: 21% 21% 57%



- Molecule 15: Synthetic peptide (polymer)

Chain 4: 21% 21% 57%

LYS	LYS
TYR	TYR
PHE	PHE
THR	THR
GLY	GLY
SER	SER
LYS	LYS
LEU	LEU
99	100
Y13	A14

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	134.04Å 302.01Å 143.84Å 90.00° 112.55° 90.00°	Depositor
Resolution (Å)	50.01 – 3.00 50.01 – 3.00	Depositor EDS
% Data completeness (in resolution range)	100.0 (50.01-3.00) 94.1 (50.01-3.00)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.24 (at 3.01Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.180 , 0.231 0.181 , 0.232	Depositor DCC
R_{free} test set	9744 reflections (4.93%)	DCC
Wilson B-factor (Å ²)	38.1	Xtrriage
Anisotropy	0.606	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 28.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	49522	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.37% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 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: GOL, MG, EDO, CL

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	0.65	0/1945	0.56	0/2634
1	O	0.67	0/1939	0.58	0/2629
2	B	0.59	0/1944	0.56	0/2634
2	P	0.63	0/1952	0.55	0/2642
3	C	0.59	0/1904	0.57	0/2580
3	Q	0.61	0/1895	0.57	0/2570
4	D	0.56	0/1879	0.56	0/2550
4	R	0.60	0/1884	0.55	0/2558
5	E	0.58	0/1840	0.54	0/2481
5	S	0.59	0/1842	0.54	0/2482
6	F	0.58	0/1799	0.54	0/2433
6	T	0.59	0/1803	0.54	0/2438
7	G	0.68	0/1920	0.57	0/2597
7	U	0.67	0/1924	0.57	0/2601
8	H	0.74	0/1541	0.56	0/2087
8	V	0.72	0/1541	0.58	0/2087
9	I	0.70	0/1715	0.60	1/2326 (0.0%)
9	W	0.70	0/1715	0.61	1/2326 (0.0%)
10	J	0.69	0/1611	0.57	0/2174
10	X	0.68	0/1607	0.56	0/2170
11	K	0.66	0/1591	0.56	0/2145
11	Y	0.69	0/1594	0.59	0/2149
12	L	0.67	0/1677	0.53	0/2270
12	Z	0.68	0/1681	0.56	0/2274
13	1	0.66	0/1791	0.55	0/2416
13	M	0.67	0/1783	0.54	0/2408
14	2	0.70	0/1855	0.58	0/2514
14	N	0.71	0/1848	0.60	0/2504
15	3	0.57	0/53	0.54	0/69
15	4	0.54	0/53	0.48	0/69
All	All	0.65	0/50126	0.56	2/67817 (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
7	U	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	I	170	GLY	N-CA-C	-6.19	97.62	113.10
9	W	170	GLY	N-CA-C	-5.32	99.79	113.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
7	U	180	ASP	Peptide

5.2 Too-close contacts ⓘ

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	1901	65	1
1	O	1901	0	1882	69	0
2	B	1907	0	1907	66	0
2	P	1915	0	1929	56	1
3	C	1875	0	1853	63	0
3	Q	1866	0	1832	62	0
4	D	1850	0	1810	67	0
4	R	1855	0	1827	59	0
5	E	1815	0	1788	68	0
5	S	1818	0	1796	60	0
6	F	1772	0	1766	57	0
6	T	1776	0	1771	61	0
7	G	1880	0	1849	55	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	U	1884	0	1860	49	0
8	H	1512	0	1481	37	0
8	V	1512	0	1481	48	0
9	I	1684	0	1688	46	0
9	W	1684	0	1688	51	0
10	J	1581	0	1574	48	0
10	X	1577	0	1563	42	0
11	K	1563	0	1569	53	0
11	Y	1566	0	1571	60	0
12	L	1640	0	1584	55	0
12	Z	1644	0	1595	40	0
13	1	1753	0	1700	55	0
13	M	1745	0	1678	42	0
14	2	1824	0	1832	37	0
14	N	1817	0	1825	40	0
15	3	52	0	42	6	0
15	4	52	0	42	3	0
16	2	3	0	0	0	0
16	A	1	0	0	0	0
16	K	2	0	0	0	0
16	N	1	0	0	0	0
16	O	1	0	0	0	0
16	R	1	0	0	0	0
16	S	1	0	0	0	0
16	V	2	0	0	0	0
17	C	1	0	0	0	0
17	D	1	0	0	0	0
17	H	1	0	0	0	0
17	I	1	0	0	0	0
17	J	1	0	0	0	0
17	N	2	0	0	0	0
17	Q	1	0	0	0	0
18	1	4	6	6	0	0
18	2	4	6	6	0	0
18	C	4	6	6	2	0
18	F	4	6	6	1	0
18	G	4	6	6	1	0
18	I	4	6	6	0	0
18	L	4	6	6	0	0
18	M	4	6	6	0	0
18	O	8	12	12	2	0
18	U	4	6	6	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	W	12	18	18	0	0
18	Y	8	12	12	1	0
19	K	6	0	8	0	0
19	L	6	0	8	0	0
19	M	6	8	8	0	0
19	Q	6	0	8	2	0
19	V	6	0	8	2	0
19	Z	12	0	16	0	0
20	1	9	0	0	1	0
20	2	8	0	0	0	0
20	A	2	0	0	2	0
20	C	2	0	0	0	0
20	D	1	0	0	0	0
20	G	2	0	0	0	0
20	H	8	0	0	1	0
20	I	2	0	0	0	0
20	J	1	0	0	0	0
20	L	1	0	0	0	0
20	M	4	0	0	0	0
20	N	4	0	0	0	0
20	O	4	0	0	0	0
20	U	2	0	0	0	0
20	V	4	0	0	0	0
20	W	3	0	0	0	0
20	X	2	0	0	0	0
20	Z	6	0	0	0	0
All	All	49418	104	48836	1366	1

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 14.

The worst 5 of 1366 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)
1:O:101:ALA:HA	1:O:112:MET:HE2	1.24	1.18
3:C:201:THR:HG22	3:C:203:SER:H	1.13	1.09
5:E:248:ALA:HA	5:E:249:ALA:HB3	1.33	1.09
1:A:101:ALA:HA	1:A:112:MET:HE2	1.45	0.98
4:R:207:ALA:HB2	4:R:233:VAL:HG21	1.44	0.98

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:185:HIS:ND1	2:P:201:GLU:OE2[2_546]	2.00	0.20

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	239/252 (95%)	230 (96%)	9 (4%)	0	100	100
1	O	240/252 (95%)	232 (97%)	8 (3%)	0	100	100
2	B	248/250 (99%)	234 (94%)	13 (5%)	1 (0%)	39	80
2	P	248/250 (99%)	235 (95%)	12 (5%)	1 (0%)	39	80
3	C	237/258 (92%)	221 (93%)	16 (7%)	0	100	100
3	Q	238/258 (92%)	223 (94%)	15 (6%)	0	100	100
4	D	239/254 (94%)	227 (95%)	11 (5%)	1 (0%)	39	80
4	R	239/254 (94%)	225 (94%)	12 (5%)	2 (1%)	24	66
5	E	232/260 (89%)	221 (95%)	11 (5%)	0	100	100
5	S	232/260 (89%)	219 (94%)	13 (6%)	0	100	100
6	F	230/234 (98%)	213 (93%)	17 (7%)	0	100	100
6	T	230/234 (98%)	215 (94%)	15 (6%)	0	100	100
7	G	242/288 (84%)	226 (93%)	16 (7%)	0	100	100
7	U	242/288 (84%)	224 (93%)	17 (7%)	1 (0%)	39	80
8	H	194/215 (90%)	186 (96%)	8 (4%)	0	100	100
8	V	194/215 (90%)	187 (96%)	7 (4%)	0	100	100
9	I	220/261 (84%)	210 (96%)	9 (4%)	1 (0%)	34	76
9	W	220/261 (84%)	212 (96%)	7 (3%)	1 (0%)	34	76
10	J	202/205 (98%)	196 (97%)	6 (3%)	0	100	100
10	X	202/205 (98%)	196 (97%)	6 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	K	194/198 (98%)	179 (92%)	12 (6%)	3 (2%)	13	50
11	Y	194/198 (98%)	181 (93%)	11 (6%)	2 (1%)	19	61
12	L	210/287 (73%)	202 (96%)	7 (3%)	1 (0%)	34	76
12	Z	210/287 (73%)	204 (97%)	6 (3%)	0	100	100
13	1	220/241 (91%)	208 (94%)	12 (6%)	0	100	100
13	M	220/241 (91%)	207 (94%)	13 (6%)	0	100	100
14	2	231/266 (87%)	220 (95%)	11 (5%)	0	100	100
14	N	230/266 (86%)	218 (95%)	12 (5%)	0	100	100
15	3	4/14 (29%)	4 (100%)	0	0	100	100
15	4	4/14 (29%)	3 (75%)	1 (25%)	0	100	100
All	All	6285/6966 (90%)	5958 (95%)	313 (5%)	14 (0%)	52	88

5 of 14 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	53	LYS
11	K	50	GLY
4	R	241	GLN
4	R	240	LYS
9	I	91	GLN

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	206/210 (98%)	199 (97%)	7 (3%)	44	81
1	O	203/210 (97%)	196 (97%)	7 (3%)	44	81
2	B	207/209 (99%)	204 (99%)	3 (1%)	74	93
2	P	209/209 (100%)	208 (100%)	1 (0%)	92	98
3	C	199/216 (92%)	197 (99%)	2 (1%)	82	95
3	Q	196/216 (91%)	195 (100%)	1 (0%)	92	98

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	D	202/226 (89%)	197 (98%)	5 (2%)	55	86
4	R	204/226 (90%)	202 (99%)	2 (1%)	82	95
5	E	193/215 (90%)	191 (99%)	2 (1%)	82	95
5	S	194/215 (90%)	193 (100%)	1 (0%)	92	98
6	F	189/193 (98%)	186 (98%)	3 (2%)	70	92
6	T	189/193 (98%)	184 (97%)	5 (3%)	54	85
7	G	197/239 (82%)	190 (96%)	7 (4%)	42	79
7	U	198/239 (83%)	194 (98%)	4 (2%)	63	89
8	H	162/178 (91%)	159 (98%)	3 (2%)	65	90
8	V	162/178 (91%)	161 (99%)	1 (1%)	90	97
9	I	181/214 (85%)	180 (99%)	1 (1%)	90	97
9	W	181/214 (85%)	179 (99%)	2 (1%)	80	94
10	J	172/173 (99%)	170 (99%)	2 (1%)	78	94
10	X	171/173 (99%)	168 (98%)	3 (2%)	66	91
11	K	172/175 (98%)	167 (97%)	5 (3%)	50	84
11	Y	173/175 (99%)	170 (98%)	3 (2%)	68	91
12	L	168/235 (72%)	165 (98%)	3 (2%)	66	91
12	Z	169/235 (72%)	167 (99%)	2 (1%)	78	94
13	1	184/201 (92%)	183 (100%)	1 (0%)	92	98
13	M	182/201 (90%)	176 (97%)	6 (3%)	45	82
14	2	199/224 (89%)	197 (99%)	2 (1%)	82	95
14	N	198/224 (88%)	196 (99%)	2 (1%)	82	95
15	3	4/12 (33%)	4 (100%)	0	100	100
15	4	4/12 (33%)	4 (100%)	0	100	100
All	All	5268/5840 (90%)	5182 (98%)	86 (2%)	70	92

5 of 86 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
11	K	62	ASN
13	M	127	CYS
11	Y	34	THR
12	L	17	ASP
13	M	25	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
13	M	143	ASN
9	W	189	ASN
14	N	70	ASN
5	E	114	GLN
3	Q	173	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](#)

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 43 ligands modelled in this entry, 20 are monoatomic - leaving 23 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	$\# Z > 2$
18	EDO	1	301	-	3,3,3	0.42	0	2,2,2	0.39	0
18	EDO	2	304	-	3,3,3	0.35	0	2,2,2	0.56	0
18	EDO	C	302	-	3,3,3	0.35	0	2,2,2	0.58	0
18	EDO	F	301	-	3,3,3	0.32	0	2,2,2	0.55	0
18	EDO	G	301	-	3,3,3	0.34	0	2,2,2	0.53	0
18	EDO	I	302	-	3,3,3	0.39	0	2,2,2	0.46	0
19	GOL	K	203	-	5,5,5	0.44	0	5,5,5	0.37	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	GOL	L	301	-	5,5,5	0.46	0	5,5,5	0.23	0
18	EDO	L	302	-	3,3,3	0.39	0	2,2,2	0.41	0
19	GOL	M	301	-	5,5,5	0.46	0	5,5,5	0.22	0
18	EDO	M	302	-	3,3,3	0.34	0	2,2,2	0.38	0
18	EDO	O	302	-	3,3,3	0.43	0	2,2,2	0.48	0
18	EDO	O	303	-	3,3,3	0.43	0	2,2,2	0.31	0
19	GOL	Q	301	-	5,5,5	0.35	0	5,5,5	0.25	0
18	EDO	U	301	-	3,3,3	0.29	0	2,2,2	0.65	0
19	GOL	V	203	-	5,5,5	0.40	0	5,5,5	0.33	0
18	EDO	W	301	-	3,3,3	0.45	0	2,2,2	0.24	0
18	EDO	W	302	-	3,3,3	0.36	0	2,2,2	0.41	0
18	EDO	W	303	-	3,3,3	0.44	0	2,2,2	0.34	0
18	EDO	Y	201	-	3,3,3	0.42	0	2,2,2	0.20	0
18	EDO	Y	202	-	3,3,3	0.32	0	2,2,2	0.73	0
19	GOL	Z	301	-	5,5,5	0.43	0	5,5,5	0.22	0
19	GOL	Z	302	-	5,5,5	0.47	0	5,5,5	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
18	EDO	1	301	-	-	0/1/1/1	0/0/0/0
18	EDO	2	304	-	-	0/1/1/1	0/0/0/0
18	EDO	C	302	-	-	0/1/1/1	0/0/0/0
18	EDO	F	301	-	-	0/1/1/1	0/0/0/0
18	EDO	G	301	-	-	0/1/1/1	0/0/0/0
18	EDO	I	302	-	-	0/1/1/1	0/0/0/0
19	GOL	K	203	-	-	0/4/4/4	0/0/0/0
19	GOL	L	301	-	-	0/4/4/4	0/0/0/0
18	EDO	L	302	-	-	0/1/1/1	0/0/0/0
19	GOL	M	301	-	-	0/4/4/4	0/0/0/0
18	EDO	M	302	-	-	0/1/1/1	0/0/0/0
18	EDO	O	302	-	-	0/1/1/1	0/0/0/0
18	EDO	O	303	-	-	0/1/1/1	0/0/0/0
19	GOL	Q	301	-	-	0/4/4/4	0/0/0/0
18	EDO	U	301	-	-	0/1/1/1	0/0/0/0
19	GOL	V	203	-	-	0/4/4/4	0/0/0/0
18	EDO	W	301	-	-	0/1/1/1	0/0/0/0
18	EDO	W	302	-	-	0/1/1/1	0/0/0/0
18	EDO	W	303	-	-	0/1/1/1	0/0/0/0
18	EDO	Y	201	-	-	0/1/1/1	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	EDO	Y	202	-	-	0/1/1/1	0/0/0/0
19	GOL	Z	301	-	-	0/4/4/4	0/0/0/0
19	GOL	Z	302	-	-	0/4/4/4	0/0/0/0

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.

7 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	C	302	EDO	2	0
18	F	301	EDO	1	0
18	G	301	EDO	1	0
18	O	302	EDO	2	0
19	Q	301	GOL	2	0
19	V	203	GOL	2	0
18	Y	201	EDO	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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	241/252 (95%)	-0.74	0 100 100	10, 22, 42, 60	0
1	O	242/252 (96%)	-0.75	1 (0%) 93 80	9, 20, 45, 85	0
2	B	250/250 (100%)	-0.62	0 100 100	12, 26, 56, 69	0
2	P	250/250 (100%)	-0.71	0 100 100	10, 21, 46, 68	0
3	C	241/258 (93%)	-0.61	0 100 100	12, 26, 54, 82	0
3	Q	242/258 (93%)	-0.69	0 100 100	12, 26, 53, 74	0
4	D	241/254 (94%)	-0.40	1 (0%) 93 80	14, 34, 77, 105	0
4	R	241/254 (94%)	-0.47	0 100 100	12, 30, 76, 106	0
5	E	236/260 (90%)	-0.65	0 100 100	13, 29, 53, 72	0
5	S	236/260 (90%)	-0.71	0 100 100	14, 25, 46, 69	0
6	F	232/234 (99%)	-0.62	0 100 100	14, 27, 45, 64	0
6	T	232/234 (99%)	-0.62	0 100 100	13, 27, 47, 63	0
7	G	244/288 (84%)	-0.70	0 100 100	8, 21, 47, 75	0
7	U	244/288 (84%)	-0.67	0 100 100	11, 23, 49, 71	0
8	H	196/215 (91%)	-0.83	0 100 100	10, 16, 32, 49	0
8	V	196/215 (91%)	-0.80	0 100 100	9, 15, 31, 55	0
9	I	222/261 (85%)	-0.76	1 (0%) 91 76	10, 20, 34, 104	0
9	W	222/261 (85%)	-0.78	0 100 100	8, 18, 35, 89	0
10	J	204/205 (99%)	-0.80	0 100 100	11, 20, 35, 60	0
10	X	204/205 (99%)	-0.77	0 100 100	9, 20, 36, 53	0
11	K	196/198 (98%)	-0.77	0 100 100	11, 20, 32, 65	0
11	Y	196/198 (98%)	-0.78	1 (0%) 91 76	11, 21, 35, 75	0
12	L	212/287 (73%)	-0.73	0 100 100	12, 22, 36, 52	0
12	Z	212/287 (73%)	-0.74	0 100 100	10, 21, 36, 51	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9	
13	1	222/241 (92%)	-0.74	0	100	100	10, 20, 38, 54	0
13	M	222/241 (92%)	-0.71	0	100	100	8, 20, 40, 59	0
14	2	233/266 (87%)	-0.80	0	100	100	8, 17, 29, 40	0
14	N	232/266 (87%)	-0.85	0	100	100	7, 16, 28, 38	0
15	3	6/14 (42%)	-0.18	0	100	100	28, 37, 49, 57	0
15	4	6/14 (42%)	-0.14	0	100	100	32, 50, 54, 55	0
All	All	6353/6966 (91%)	-0.70	4 (0%)	95	90	7, 22, 48, 106	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	O	10	ALA	3.4
9	I	222	ASP	2.8
11	Y	195	GLN	2.5
4	D	51	THR	2.1

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

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, 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
19	GOL	Q	301	6/6	0.88	0.33	12.79	19,28,31,36	0
19	GOL	V	203	6/6	0.95	0.28	7.90	20,22,34,35	0
18	EDO	U	301	4/4	0.94	0.29	6.10	25,31,38,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
18	EDO	2	304	4/4	0.94	0.35	5.95	30,36,41,41	0
18	EDO	W	303	4/4	0.76	0.25	5.21	30,38,49,49	0
18	EDO	O	302	4/4	0.94	0.24	4.53	22,26,30,30	0
18	EDO	G	301	4/4	0.96	0.23	4.50	24,30,37,45	0
18	EDO	C	302	4/4	0.95	0.28	4.40	23,28,35,42	0
18	EDO	Y	202	4/4	0.83	0.22	4.23	33,40,50,60	0
18	EDO	O	303	4/4	0.93	0.20	3.50	23,27,33,33	0
18	EDO	L	302	4/4	0.89	0.26	2.77	22,27,30,30	0
19	GOL	L	301	6/6	0.92	0.20	2.36	21,29,32,36	0
19	GOL	K	203	6/6	0.91	0.22	2.20	24,35,39,39	0
18	EDO	Y	201	4/4	0.88	0.22	1.73	23,35,46,46	0
18	EDO	M	302	4/4	0.96	0.32	1.57	20,24,27,27	0
18	EDO	I	302	4/4	0.94	0.19	1.56	24,38,52,52	0
19	GOL	Z	301	6/6	0.89	0.19	1.44	25,38,41,43	0
19	GOL	Z	302	6/6	0.95	0.20	0.81	15,24,28,28	0
18	EDO	F	301	4/4	0.98	0.14	-0.02	19,23,23,26	0
18	EDO	W	302	4/4	0.96	0.13	-0.47	24,29,30,34	0
16	CL	A	301	1/1	0.92	0.10	-0.93	34,34,34,34	0
17	MG	N	303	1/1	0.98	0.07	-3.55	20,20,20,20	0
16	CL	2	302	1/1	0.98	0.07	-3.98	29,29,29,29	0
16	CL	O	301	1/1	0.91	0.14	-	27,27,27,27	0
16	CL	N	301	1/1	0.97	0.14	-	31,31,31,31	0
16	CL	V	202	1/1	0.87	0.13	-	28,28,28,28	0
16	CL	S	301	1/1	0.98	0.06	-	28,28,28,28	0
16	CL	2	301	1/1	0.77	0.20	-	41,41,41,41	0
16	CL	K	202	1/1	0.93	0.11	-	27,27,27,27	0
17	MG	C	301	1/1	0.94	0.12	-	15,15,15,15	0
17	MG	J	201	1/1	0.94	0.14	-	15,15,15,15	0
18	EDO	1	301	4/4	0.89	0.23	-	22,31,38,38	0
17	MG	D	301	1/1	0.95	0.10	-	17,17,17,17	0
16	CL	K	201	1/1	0.92	0.10	-	29,29,29,29	0
16	CL	2	303	1/1	0.97	0.08	-	36,36,36,36	0
17	MG	N	302	1/1	0.83	0.14	-	18,18,18,18	0
16	CL	V	201	1/1	0.95	0.07	-	27,27,27,27	0
16	CL	R	301	1/1	0.95	0.12	-	46,46,46,46	0
17	MG	I	301	1/1	0.93	0.13	-	20,20,20,20	0
17	MG	Q	302	1/1	0.96	0.10	-	16,16,16,16	0
19	GOL	M	301	6/6	0.96	0.21	-	26,35,40,46	0
18	EDO	W	301	4/4	0.85	0.20	-	23,31,38,38	0
17	MG	H	201	1/1	0.96	0.09	-	15,15,15,15	0

6.5 Other polymers [i](#)

There are no such residues in this entry.