Full wwPDB X-ray Structure Validation Report (i)

Jan 2, 2024 – 10:54 pm GMT

PDB ID	:	5L5W
Title	:	Yeast 20S proteasome with human beta5c (1-138) and human beta6 (97-111; 118-133)
Authors	:	Groll, M.; Huber, E.M.
Deposited on	:	2016-05-28
Resolution	:	2.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

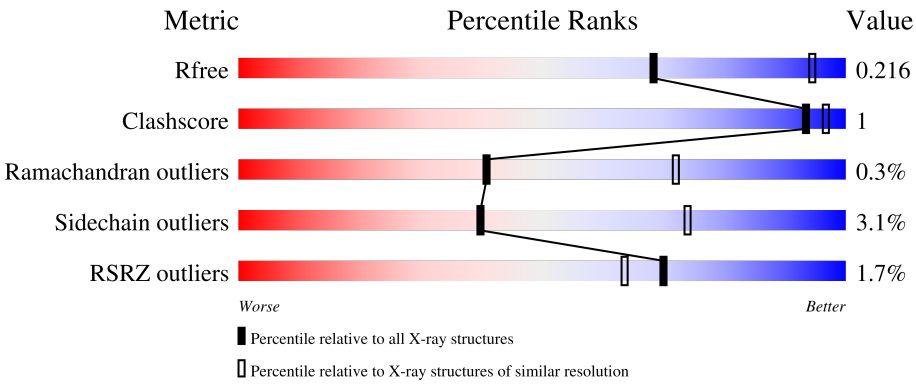
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 2.80 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}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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	2%, 98%, •
1	O	250	3%, 97%, •
2	B	258	3%, 89%, 5%, 5%
2	P	258	3%, 88%, 5%, •, 5%
3	C	254	4%, 87%, 6%, •, 6%

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Mol	Chain	Length	Quality of chain
3	Q	254	5% 87% 6% 6%
4	D	260	86% 10%
4	R	260	2% 86% 10%
5	E	234	94%
5	S	234	% 95%
6	F	288	2% 81% 16%
6	T	288	% 81% 16%
7	G	252	2% 91% 5%
7	U	252	% 90% 5%
8	H	232	2% 93%
8	V	232	2% 93%
9	I	205	95% 5%
9	W	205	92% 7%
10	J	198	2% 92% 7%
10	X	198	2% 92% 7%
11	K	211	84% 13%
11	Y	211	% 84% 13%
12	L	222	% 93% 6%
12	Z	222	2% 94% 5%
13	M	246	90% 5%
13	a	246	92% 5%
14	N	196	93% 5%
14	b	196	% 97%

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	MG	M	301	-	-	-	X

2 Entry composition (i)

There are 17 unique types of molecules in this entry. The entry contains 49684 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 subunit alpha type-2.

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

- Molecule 2 is a protein called Proteasome subunit alpha type-3.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	240	1881	1176	329	372	4	0	0	0
3	Q	240	1881	1176	329	372	4	0	0	0

- Molecule 4 is a protein called Proteasome subunit alpha type-5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	235	1813	1136	304	366	7	0	0	0
4	R	235	1813	1136	304	366	7	0	0	0

- Molecule 5 is a protein called Proteasome subunit alpha type-6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	E	231	1773	1114	307	348	4	0	0	0
5	S	231	1773	1114	307	348	4	0	0	0

- Molecule 6 is a protein called Probable proteasome subunit alpha type-7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
6	F	243	1892	1203	329	356	4	0	0	0
6	T	243	1892	1203	329	356	4	0	0	0

- Molecule 7 is a protein called Proteasome subunit alpha type-1.

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

- Molecule 8 is a protein called Proteasome subunit beta type-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
8	H	226	1719	1082	298	332	7	0	0	0
8	V	226	1719	1082	298	332	7	0	0	0

- Molecule 9 is a protein called Proteasome subunit beta type-3.

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

- Molecule 10 is a protein called Proteasome subunit beta type-4.

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

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

- Molecule 11 is a protein called Proteasome subunit beta type-5,Proteasome subunit beta type-5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
11	K	211	1632	1036	282	306	8	0	0	0
			Total	C	N	O	S			
11	Y	211	1632	1036	282	306	8	0	0	0

- Molecule 12 is a protein called Proteasome subunit beta type-6,Proteasome subunit beta type-1,Proteasome subunit beta type-6,Proteasome subunit beta type-1,Proteasome subunit beta type-6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
12	L	222	1764	1119	305	336	4	0	0	0
			Total	C	N	O	S			
12	Z	222	1764	1119	305	336	4	0	0	0

- Molecule 13 is a protein called Proteasome subunit beta type-7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
13	M	233	1824	1154	312	351	7	0	0	0
			Total	C	N	O	S			
13	a	233	1832	1159	315	351	7	0	1	0

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

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

- Molecule 15 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	E	1	Total Cl 1 1	0	0
15	G	1	Total Cl 1 1	0	0
15	U	1	Total Cl 1 1	0	0
15	b	1	Total Cl 1 1	0	0

- Molecule 16 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	G	1	Total Mg 1 1	0	0
16	H	1	Total Mg 1 1	0	0
16	I	2	Total Mg 2 2	0	0
16	J	1	Total Mg 1 1	0	0
16	K	2	Total Mg 2 2	0	0
16	L	1	Total Mg 1 1	0	0
16	M	1	Total Mg 1 1	0	0
16	N	1	Total Mg 1 1	0	0
16	Z	1	Total Mg 1 1	0	0
16	b	1	Total Mg 1 1	0	0

- Molecule 17 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	A	10	Total O 10 10	0	0
17	B	11	Total O 11 11	0	0
17	C	10	Total O 10 10	0	0
17	D	6	Total O 6 6	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	E	5	Total O 5 5	0	0
17	F	9	Total O 9 9	0	0
17	G	13	Total O 13 13	0	0
17	H	11	Total O 11 11	0	0
17	I	10	Total O 10 10	0	0
17	J	7	Total O 7 7	0	0
17	K	16	Total O 16 16	0	0
17	L	14	Total O 14 14	0	0
17	M	16	Total O 16 16	0	0
17	N	12	Total O 12 12	0	0
17	O	6	Total O 6 6	0	0
17	P	9	Total O 9 9	0	0
17	Q	11	Total O 11 11	0	0
17	R	13	Total O 13 13	0	0
17	S	11	Total O 11 11	0	0
17	T	8	Total O 8 8	0	0
17	U	17	Total O 17 17	0	0
17	V	16	Total O 16 16	0	0
17	W	13	Total O 13 13	0	0
17	X	6	Total O 6 6	0	0
17	Y	15	Total O 15 15	0	0

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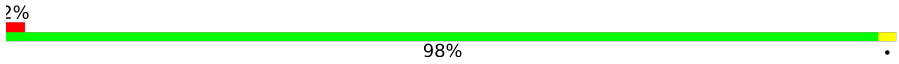
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
17	Z	4	4	4	0	0
			Total	O		
17	a	13	13	13	0	0
			Total	O		
17	b	12	12	12	0	0

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.

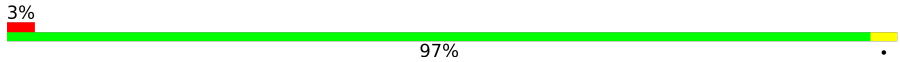
• Molecule 1: Proteasome subunit alpha type-2

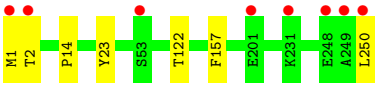
Chain A:



• Molecule 1: Proteasome subunit alpha type-2

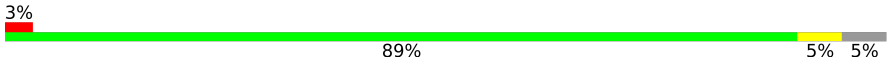
Chain O:

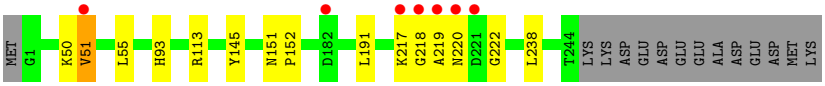




• Molecule 2: Proteasome subunit alpha type-3

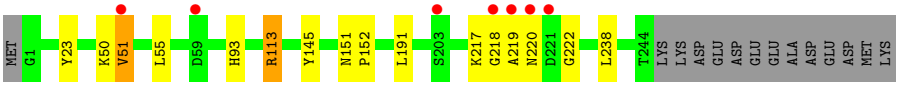
Chain B:





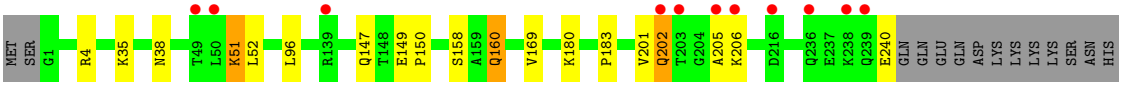
• Molecule 2: Proteasome subunit alpha type-3

Chain P:



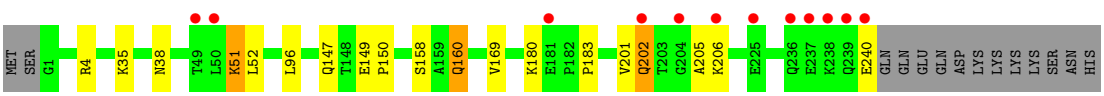
• Molecule 3: Proteasome subunit alpha type-4

Chain C:



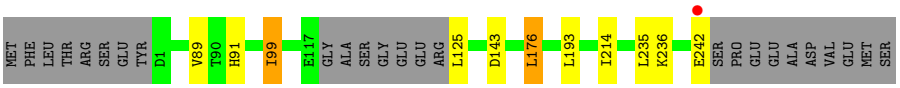
• Molecule 3: Proteasome subunit alpha type-4

Chain Q:



• Molecule 4: Proteasome subunit alpha type-5

Chain D:

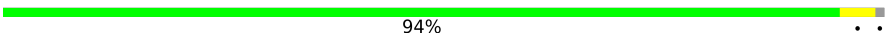


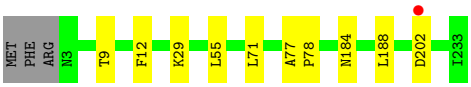
• Molecule 4: Proteasome subunit alpha type-5

Chain R:

• Molecule 5: Proteasome subunit alpha type-6

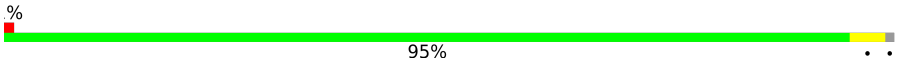
Chain E:

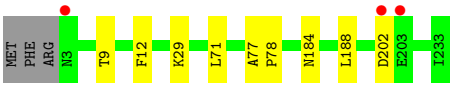




• Molecule 5: Proteasome subunit alpha type-6

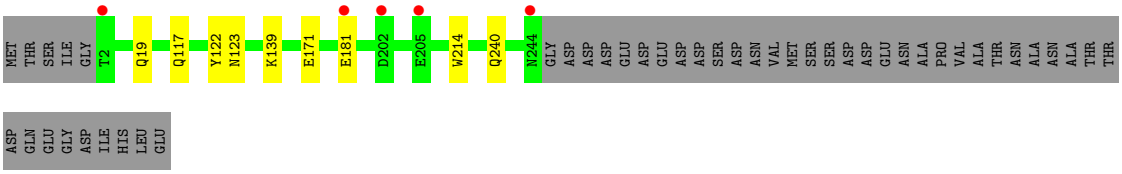
Chain S:





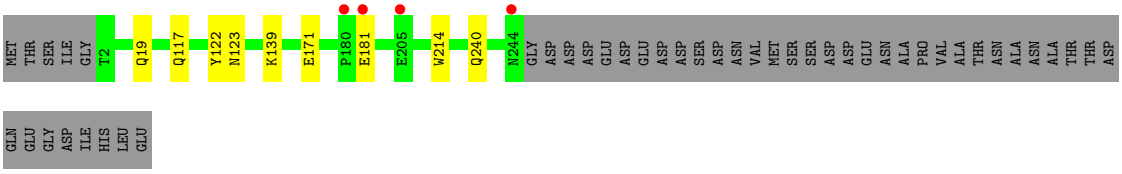
• Molecule 6: Probable proteasome subunit alpha type-7

Chain F:



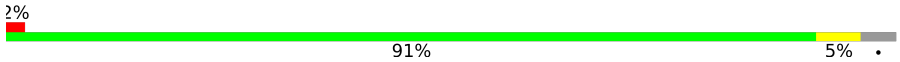
• Molecule 6: Probable proteasome subunit alpha type-7

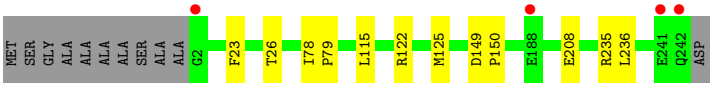
Chain T:



• Molecule 7: Proteasome subunit alpha type-1

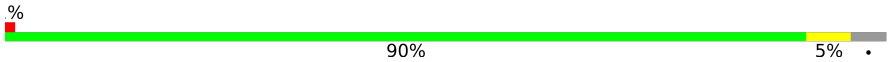
Chain G:

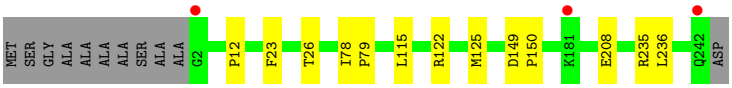




• Molecule 7: Proteasome subunit alpha type-1

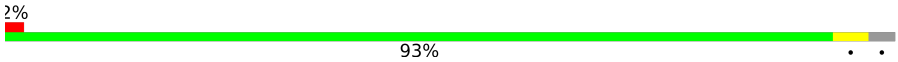
Chain U:





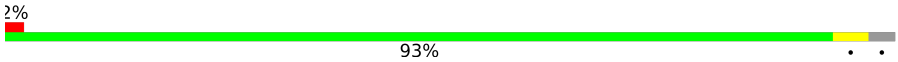
• Molecule 8: Proteasome subunit beta type-2

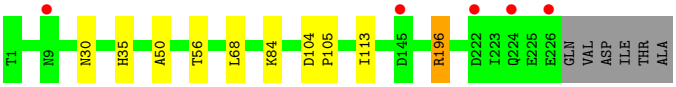
Chain H:



• Molecule 8: Proteasome subunit beta type-2

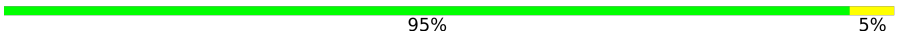
Chain V:

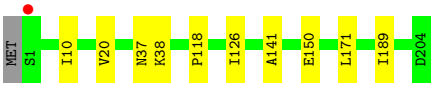




• Molecule 9: Proteasome subunit beta type-3

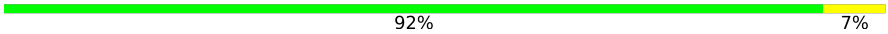
Chain I:

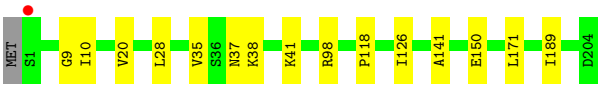




• Molecule 9: Proteasome subunit beta type-3

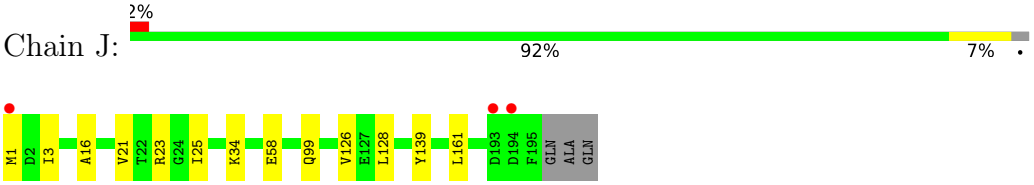
Chain W:





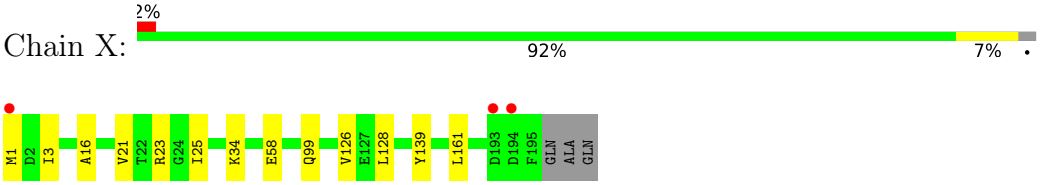
• Molecule 10: Proteasome subunit beta type-4

Chain J:



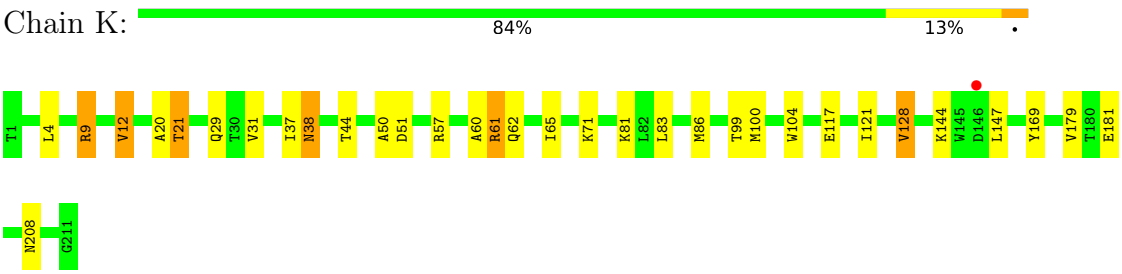
• Molecule 10: Proteasome subunit beta type-4

Chain X:



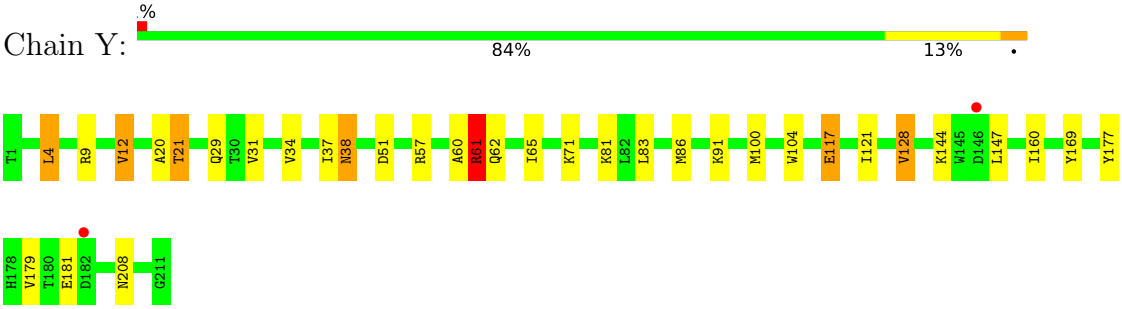
• Molecule 11: Proteasome subunit beta type-5,Proteasome subunit beta type-5

Chain K:



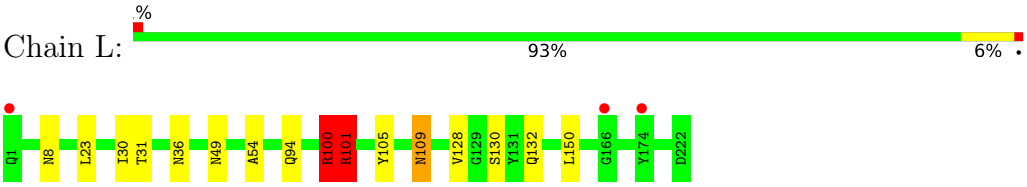
• Molecule 11: Proteasome subunit beta type-5,Proteasome subunit beta type-5

Chain Y:



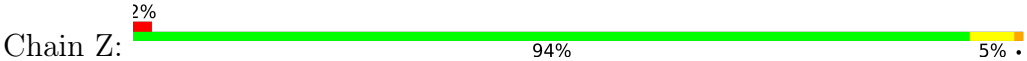
• Molecule 12: Proteasome subunit beta type-6,Proteasome subunit beta type-1,Proteasome subunit beta type-6,Proteasome subunit beta type-1,Proteasome subunit beta type-6

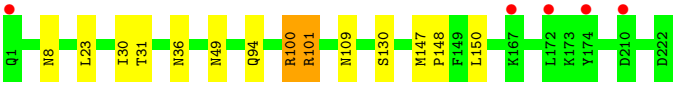
Chain L:



• Molecule 12: Proteasome subunit beta type-6,Proteasome subunit beta type-1,Proteasome subunit beta type-6,Proteasome subunit beta type-1,Proteasome subunit beta type-6

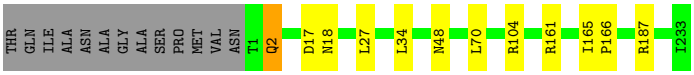
Chain Z:





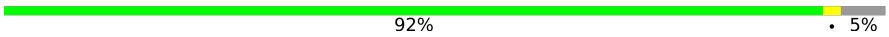
• Molecule 13: Proteasome subunit beta type-7

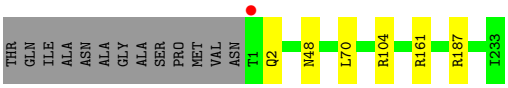
Chain M:



• Molecule 13: Proteasome subunit beta type-7

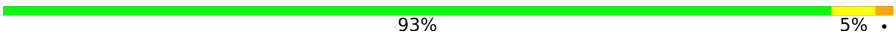
Chain a:

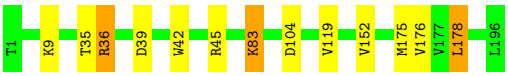




• Molecule 14: Proteasome subunit beta type-1

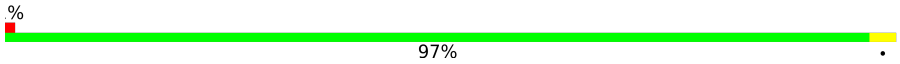
Chain N:

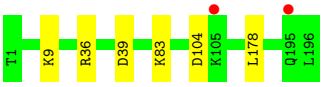




• Molecule 14: Proteasome subunit beta type-1

Chain b:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	135.07Å 300.35Å 145.24Å 90.00° 112.50° 90.00°	Depositor
Resolution (Å)	15.00 – 2.80 15.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	97.9 (15.00-2.80) 97.9 (15.00-2.80)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.77 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.185 , 0.212 0.192 , 0.216	Depositor DCC
R_{free} test set	12718 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	55.0	Xtriage
Anisotropy	0.149	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 38.8	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	49684	wwPDB-VP
Average B, all atoms (Å^2)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.36% 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: MG, 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	0.27	0/1952	0.46	0/2642
1	O	0.27	0/1952	0.46	0/2642
2	B	0.28	0/1934	0.49	0/2618
2	P	0.28	0/1934	0.49	0/2618
3	C	0.28	0/1910	0.50	0/2586
3	Q	0.28	0/1910	0.50	0/2586
4	D	0.27	0/1837	0.47	0/2475
4	R	0.27	0/1837	0.47	0/2475
5	E	0.27	0/1800	0.47	0/2433
5	S	0.27	0/1800	0.47	0/2433
6	F	0.28	0/1932	0.45	0/2609
6	T	0.27	0/1932	0.45	0/2609
7	G	0.27	0/1945	0.47	0/2634
7	U	0.27	0/1945	0.47	0/2634
8	H	0.25	0/1750	0.49	0/2373
8	V	0.25	0/1750	0.48	0/2373
9	I	0.27	0/1611	0.51	0/2174
9	W	0.27	0/1611	0.51	0/2174
10	J	0.27	0/1589	0.48	0/2142
10	X	0.27	0/1589	0.48	0/2142
11	K	0.29	0/1668	0.62	2/2253 (0.1%)
11	Y	0.28	0/1668	0.62	2/2253 (0.1%)
12	L	0.38	2/1802 (0.1%)	0.89	6/2430 (0.2%)
12	Z	0.37	2/1802 (0.1%)	1.01	6/2430 (0.2%)
13	M	0.27	0/1855	0.51	0/2514
13	a	0.26	0/1866	0.51	0/2528
14	N	0.25	0/1541	0.49	0/2087
14	b	0.25	0/1541	0.49	0/2087
All	All	0.28	4/50263 (0.0%)	0.54	16/67954 (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 (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	L	109	ASN	CG-ND2	-5.45	1.19	1.32
12	Z	94	GLN	CD-NE2	-5.33	1.19	1.32
12	L	94	GLN	CD-NE2	-5.23	1.19	1.32
12	Z	109	ASN	CG-ND2	-5.19	1.19	1.32

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	Z	100	ARG	NE-CZ-NH1	-22.39	109.11	120.30
12	Z	101	ARG	NE-CZ-NH2	-20.98	109.81	120.30
12	L	101	ARG	NE-CZ-NH1	-20.59	110.00	120.30
12	Z	100	ARG	NE-CZ-NH2	20.05	130.32	120.30
12	L	101	ARG	NE-CZ-NH2	18.50	129.55	120.30
12	Z	101	ARG	NE-CZ-NH1	17.80	129.20	120.30
12	L	100	ARG	NE-CZ-NH2	-15.68	112.46	120.30
12	L	100	ARG	NE-CZ-NH1	12.08	126.34	120.30
11	Y	61	ARG	CB-CG-CD	10.26	138.28	111.60
11	K	61	ARG	CB-CG-CD	10.13	137.95	111.60
12	L	101	ARG	CD-NE-CZ	9.56	136.99	123.60
12	Z	101	ARG	CD-NE-CZ	9.10	136.34	123.60
12	Z	100	ARG	CD-NE-CZ	8.87	136.02	123.60
11	K	9	ARG	CG-CD-NE	8.01	128.61	111.80
11	Y	9	ARG	CG-CD-NE	7.61	127.78	111.80
12	L	100	ARG	CD-NE-CZ	7.40	133.96	123.60

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
12	L	100	ARG	Sidechain
12	Z	100	ARG	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	1929	1	0
1	O	1915	0	1929	3	0
2	B	1904	0	1904	6	0
2	P	1904	0	1904	8	0
3	C	1881	0	1895	7	0
3	Q	1881	0	1895	7	0
4	D	1813	0	1797	6	0
4	R	1813	0	1797	2	0
5	E	1773	0	1775	3	0
5	S	1773	0	1775	2	0
6	F	1892	0	1883	2	0
6	T	1892	0	1883	2	0
7	G	1907	0	1901	3	0
7	U	1907	0	1901	4	0
8	H	1719	0	1719	8	0
8	V	1719	0	1719	7	0
9	I	1581	0	1574	7	0
9	W	1581	0	1574	10	0
10	J	1561	0	1569	7	0
10	X	1561	0	1569	7	0
11	K	1632	0	1593	21	0
11	Y	1632	0	1593	18	0
12	L	1764	0	1716	6	0
12	Z	1764	0	1716	4	0
13	M	1824	0	1832	4	0
13	a	1832	0	1845	0	0
14	N	1512	0	1481	5	0
14	b	1512	0	1481	0	0
15	E	1	0	0	0	0
15	G	1	0	0	0	0
15	U	1	0	0	0	0
15	b	1	0	0	0	0
16	G	1	0	0	0	0
16	H	1	0	0	0	0
16	I	2	0	0	0	0
16	J	1	0	0	0	0
16	K	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	L	1	0	0	0	0
16	M	1	0	0	0	0
16	N	1	0	0	0	0
16	Z	1	0	0	0	0
16	b	1	0	0	0	0
17	A	10	0	0	0	0
17	B	11	0	0	1	0
17	C	10	0	0	0	0
17	D	6	0	0	0	0
17	E	5	0	0	0	0
17	F	9	0	0	0	0
17	G	13	0	0	0	0
17	H	11	0	0	0	0
17	I	10	0	0	0	0
17	J	7	0	0	0	0
17	K	16	0	0	0	0
17	L	14	0	0	0	0
17	M	16	0	0	1	0
17	N	12	0	0	0	0
17	O	6	0	0	0	0
17	P	9	0	0	2	0
17	Q	11	0	0	0	0
17	R	13	0	0	0	0
17	S	11	0	0	0	0
17	T	8	0	0	0	0
17	U	17	0	0	0	0
17	V	16	0	0	0	0
17	W	13	0	0	0	0
17	X	6	0	0	0	0
17	Y	15	0	0	0	0
17	Z	4	0	0	0	0
17	a	13	0	0	0	0
17	b	12	0	0	0	0
All	All	49684	0	49149	129	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 1.

All (129) 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)
4:R:89:VAL:HG12	11:Y:61:ARG:HD3	1.72	0.72
4:D:89:VAL:CG1	11:K:61:ARG:HG2	2.21	0.71
4:D:89:VAL:HG12	11:K:61:ARG:HG2	1.74	0.70
14:N:152:VAL:HA	14:N:175:MET:HE1	1.85	0.58
8:V:35:HIS:HB3	8:V:56:THR:HG21	1.86	0.58
8:H:35:HIS:HB3	8:H:56:THR:HG21	1.85	0.58
11:K:12:VAL:HG13	11:K:179:VAL:HB	1.88	0.56
11:Y:12:VAL:HG13	11:Y:179:VAL:HB	1.88	0.55
4:D:89:VAL:HG12	11:K:61:ARG:CG	2.36	0.55
13:M:2:GLN:NE2	17:M:401:HOH:O	2.40	0.54
10:J:16:ALA:HB2	10:J:161:LEU:HD21	1.91	0.52
11:K:104:TRP:CE2	11:K:181:GLU:HB3	2.44	0.52
3:Q:51:LYS:O	3:Q:52:LEU:HB2	2.08	0.52
8:H:196:ARG:NH2	9:I:150:GLU:O	2.42	0.52
11:Y:104:TRP:CE2	11:Y:181:GLU:HB3	2.44	0.52
10:J:126:VAL:HG12	10:J:128:LEU:HG	1.92	0.52
12:Z:31:THR:HG23	12:Z:36:ASN:HD21	1.74	0.52
7:U:23:PHE:O	7:U:26:THR:HB	2.10	0.52
10:X:16:ALA:HB2	10:X:161:LEU:HD21	1.92	0.51
3:Q:201:VAL:O	3:Q:202:GLN:CB	2.58	0.51
3:C:201:VAL:O	3:C:202:GLN:CB	2.58	0.51
3:Q:96:LEU:O	11:Y:81:LYS:HE2	2.10	0.51
3:C:51:LYS:O	3:C:52:LEU:HB2	2.09	0.51
8:H:50:ALA:CB	9:I:126:ILE:HG23	2.40	0.51
12:L:31:THR:HG23	12:L:36:ASN:HD21	1.75	0.51
10:X:126:VAL:HG12	10:X:128:LEU:HG	1.92	0.50
14:N:83:LYS:HG3	14:N:119:VAL:CG2	2.42	0.50
10:J:1:MET:HB3	10:J:34:LYS:HE3	1.93	0.50
10:X:1:MET:HB3	10:X:34:LYS:HE3	1.94	0.50
7:G:23:PHE:O	7:G:26:THR:HB	2.12	0.49
9:I:10:ILE:HG21	9:I:141:ALA:HB3	1.94	0.49
10:J:25:ILE:O	10:X:139:TYR:OH	2.30	0.49
9:W:10:ILE:HG21	9:W:141:ALA:HB3	1.94	0.49
10:J:139:TYR:OH	10:X:25:ILE:O	2.30	0.49
11:K:208:ASN:O	9:W:38:LYS:NZ	2.46	0.48
2:B:93:HIS:HB3	17:B:301:HOH:O	2.14	0.48
2:P:113:ARG:NE	17:P:301:HOH:O	2.34	0.48
8:H:35:HIS:CB	8:H:56:THR:HG21	2.44	0.47
11:Y:37:ILE:HG23	11:Y:60:ALA:HB2	1.96	0.47
8:H:84:LYS:HA	8:H:113:ILE:HD11	1.97	0.47
8:V:50:ALA:CB	9:W:126:ILE:HG23	2.45	0.47
8:V:196:ARG:NH2	9:W:150:GLU:O	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:201:VAL:O	3:Q:202:GLN:HB3	2.15	0.47
8:V:35:HIS:CB	8:V:56:THR:HG21	2.45	0.47
3:C:201:VAL:O	3:C:202:GLN:HB3	2.15	0.47
8:H:196:ARG:NH2	9:I:150:GLU:HG3	2.30	0.47
9:I:20:VAL:HG23	9:I:189:ILE:HB	1.96	0.47
11:K:37:ILE:HG23	11:K:60:ALA:HB2	1.96	0.47
2:P:93:HIS:HB3	17:P:301:HOH:O	2.16	0.46
9:W:20:VAL:HG23	9:W:189:ILE:HB	1.96	0.46
8:H:104:ASP:HB2	8:H:105:PRO:HD2	1.98	0.46
10:J:58:GLU:OE1	11:K:81:LYS:NZ	2.47	0.46
3:Q:160:GLN:HE21	3:Q:160:GLN:HA	1.81	0.46
11:Y:100:MET:SD	11:Y:128:VAL:CG1	3.03	0.46
1:O:23:TYR:CD1	7:U:12:PRO:HA	2.50	0.46
12:L:54:ALA:HB2	12:L:109:ASN:OD1	2.16	0.46
11:K:100:MET:SD	11:K:128:VAL:CG1	3.04	0.45
11:K:51:ASP:OD2	12:L:101:ARG:NH2	2.49	0.45
3:C:160:GLN:HE21	3:C:160:GLN:HA	1.81	0.45
8:V:84:LYS:HA	8:V:113:ILE:HD11	1.97	0.45
8:V:104:ASP:HB2	8:V:105:PRO:HD2	1.98	0.45
9:I:38:LYS:NZ	11:Y:208:ASN:O	2.50	0.45
10:X:58:GLU:OE1	11:Y:81:LYS:NZ	2.49	0.45
11:K:20:ALA:HB2	11:K:31:VAL:HG21	1.99	0.45
3:C:35:LYS:HG2	3:C:158:SER:O	2.18	0.44
1:O:1:MET:HG3	6:T:122:TYR:CZ	2.52	0.44
2:B:50:LYS:O	2:B:51:VAL:C	2.56	0.44
14:N:176:VAL:HG12	14:N:178:LEU:HD13	1.98	0.44
2:B:145:TYR:OH	2:B:217:LYS:N	2.51	0.44
9:I:20:VAL:HG13	9:I:118:PRO:HB3	2.00	0.44
2:P:50:LYS:O	2:P:51:VAL:C	2.56	0.44
3:Q:35:LYS:HG2	3:Q:158:SER:O	2.18	0.44
9:W:20:VAL:HG13	9:W:118:PRO:HB3	1.99	0.44
11:Y:61:ARG:O	11:Y:65:ILE:HG13	2.17	0.44
11:Y:20:ALA:HB2	11:Y:31:VAL:HG21	1.99	0.43
11:Y:38:ASN:OD1	11:Y:38:ASN:C	2.57	0.43
11:K:61:ARG:O	11:K:65:ILE:HG13	2.19	0.43
7:G:149:ASP:HB2	7:G:150:PRO:CD	2.49	0.43
4:D:91:HIS:HB3	4:D:99:ILE:CG2	2.48	0.43
7:U:149:ASP:HB2	7:U:150:PRO:CD	2.49	0.43
14:N:35:THR:HG21	14:N:45:ARG:HE	1.84	0.43
2:B:217:LYS:C	2:B:219:ALA:H	2.22	0.43
2:P:145:TYR:OH	2:P:217:LYS:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:176:LEU:HD22	5:E:55:LEU:CD2	2.49	0.42
3:C:149:GLU:HB2	3:C:150:PRO:HD2	2.01	0.42
11:K:50:ALA:CB	12:L:128:VAL:HG23	2.49	0.42
8:V:196:ARG:NH2	9:W:150:GLU:HG3	2.33	0.42
9:W:28:LEU:HD23	9:W:35:VAL:HB	2.02	0.42
11:Y:91:LYS:HE3	11:Y:117:GLU:O	2.20	0.42
7:G:78:ILE:N	7:G:79:PRO:CD	2.83	0.42
5:S:12:PHE:H	6:T:19:GLN:HE22	1.67	0.42
12:L:8:ASN:HA	12:L:30:ILE:O	2.20	0.42
12:L:100:ARG:HD3	12:L:105:TYR:CZ	2.54	0.42
12:Z:8:ASN:HA	12:Z:30:ILE:O	2.20	0.42
10:J:21:VAL:HG11	11:K:121:ILE:HD11	2.01	0.42
11:K:38:ASN:OD1	11:K:38:ASN:C	2.57	0.42
14:N:36:ARG:HG3	14:N:42:TRP:CE2	2.55	0.42
4:D:89:VAL:HG11	11:K:61:ARG:HG2	2.02	0.42
4:R:91:HIS:HB3	4:R:99:ILE:CG2	2.49	0.41
9:W:98:ARG:O	9:W:126:ILE:HD11	2.20	0.41
11:Y:51:ASP:OD2	12:Z:101:ARG:NH2	2.50	0.41
1:A:1:MET:HG3	6:F:122:TYR:CZ	2.56	0.41
7:U:78:ILE:N	7:U:79:PRO:CD	2.83	0.41
2:B:151:ASN:HB2	2:B:152:PRO:CD	2.50	0.41
2:P:217:LYS:C	2:P:219:ALA:H	2.23	0.41
3:Q:149:GLU:HB2	3:Q:150:PRO:HD2	2.01	0.41
1:O:14:PRO:HA	2:P:23:TYR:CD1	2.56	0.41
5:S:77:ALA:N	5:S:78:PRO:CD	2.84	0.41
5:E:12:PHE:H	6:F:19:GLN:HE22	1.69	0.41
5:E:77:ALA:N	5:E:78:PRO:CD	2.84	0.41
2:P:151:ASN:HB2	2:P:152:PRO:CD	2.51	0.41
10:X:21:VAL:HG11	11:Y:121:ILE:HD11	2.03	0.41
13:M:27:LEU:HD21	13:M:34:LEU:HD22	2.03	0.41
8:H:84:LYS:HE2	8:H:119:THR:HG23	2.03	0.41
11:K:144:LYS:HB2	11:K:147:LEU:HD13	2.03	0.41
11:Y:4:LEU:HD13	11:Y:160:ILE:HD11	2.03	0.41
2:B:145:TYR:OH	2:B:217:LYS:HB2	2.22	0.40
11:K:21:THR:HG21	11:K:169:TYR:CD1	2.56	0.40
11:K:44:THR:O	11:K:99:THR:OG1	2.39	0.40
13:M:165:ILE:HB	13:M:166:PRO:HD3	2.04	0.40
9:W:9:GLY:HA3	9:W:41:LYS:HE2	2.03	0.40
11:Y:34:VAL:HG11	11:Y:177:TYR:CD1	2.56	0.40
11:K:9:ARG:HH21	11:K:9:ARG:HD3	1.74	0.40
13:M:17:ASP:OD1	13:M:18:ASN:N	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:50:LYS:HD3	2:P:50:LYS:HA	1.89	0.40
11:Y:21:THR:HG21	11:Y:169:TYR:CD1	2.56	0.40
12:Z:147:MET:N	12:Z:148:PRO:CD	2.84	0.40
3:C:96:LEU:O	11:K:81:LYS:HE2	2.22	0.40
11:Y:144:LYS:HB2	11:Y:147:LEU:HD13	2.04	0.40

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%)	239 (96%)	8 (3%)	1 (0%)	34	66
1	O	248/250 (99%)	238 (96%)	9 (4%)	1 (0%)	34	66
2	B	242/258 (94%)	233 (96%)	5 (2%)	4 (2%)	9	29
2	P	242/258 (94%)	233 (96%)	5 (2%)	4 (2%)	9	29
3	C	238/254 (94%)	233 (98%)	2 (1%)	3 (1%)	12	36
3	Q	238/254 (94%)	233 (98%)	2 (1%)	3 (1%)	12	36
4	D	231/260 (89%)	227 (98%)	4 (2%)	0	100	100
4	R	231/260 (89%)	225 (97%)	6 (3%)	0	100	100
5	E	229/234 (98%)	221 (96%)	8 (4%)	0	100	100
5	S	229/234 (98%)	221 (96%)	8 (4%)	0	100	100
6	F	241/288 (84%)	239 (99%)	2 (1%)	0	100	100
6	T	241/288 (84%)	239 (99%)	2 (1%)	0	100	100
7	G	239/252 (95%)	236 (99%)	3 (1%)	0	100	100
7	U	239/252 (95%)	236 (99%)	3 (1%)	0	100	100
8	H	224/232 (97%)	220 (98%)	4 (2%)	0	100	100
8	V	224/232 (97%)	220 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	I	202/205 (98%)	195 (96%)	7 (4%)	0	100	100
9	W	202/205 (98%)	195 (96%)	7 (4%)	0	100	100
10	J	193/198 (98%)	190 (98%)	3 (2%)	0	100	100
10	X	193/198 (98%)	190 (98%)	3 (2%)	0	100	100
11	K	209/211 (99%)	202 (97%)	7 (3%)	0	100	100
11	Y	209/211 (99%)	203 (97%)	6 (3%)	0	100	100
12	L	220/222 (99%)	214 (97%)	6 (3%)	0	100	100
12	Z	220/222 (99%)	214 (97%)	6 (3%)	0	100	100
13	M	231/246 (94%)	222 (96%)	9 (4%)	0	100	100
13	a	232/246 (94%)	223 (96%)	9 (4%)	0	100	100
14	N	194/196 (99%)	187 (96%)	7 (4%)	0	100	100
14	b	194/196 (99%)	187 (96%)	7 (4%)	0	100	100
All	All	6283/6612 (95%)	6115 (97%)	152 (2%)	16 (0%)	41	72

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	51	VAL
3	C	202	GLN
2	P	51	VAL
3	Q	202	GLN
1	A	2	THR
2	B	218	GLY
2	B	222	GLY
1	O	2	THR
2	P	218	GLY
2	P	222	GLY
3	C	205	ALA
3	Q	205	ALA
2	B	220	ASN
2	P	220	ASN
3	Q	183	PRO
3	C	183	PRO

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%)	206 (99%)	3 (1%)	67	90
1	O	209/209 (100%)	206 (99%)	3 (1%)	67	90
2	B	203/216 (94%)	199 (98%)	4 (2%)	55	84
2	P	203/216 (94%)	199 (98%)	4 (2%)	55	84
3	C	212/226 (94%)	203 (96%)	9 (4%)	30	63
3	Q	212/226 (94%)	203 (96%)	9 (4%)	30	63
4	D	194/215 (90%)	185 (95%)	9 (5%)	27	60
4	R	194/215 (90%)	185 (95%)	9 (5%)	27	60
5	E	190/193 (98%)	184 (97%)	6 (3%)	39	73
5	S	190/193 (98%)	184 (97%)	6 (3%)	39	73
6	F	201/239 (84%)	194 (96%)	7 (4%)	36	70
6	T	201/239 (84%)	194 (96%)	7 (4%)	36	70
7	G	206/210 (98%)	200 (97%)	6 (3%)	42	76
7	U	206/210 (98%)	200 (97%)	6 (3%)	42	76
8	H	185/190 (97%)	182 (98%)	3 (2%)	62	88
8	V	185/190 (97%)	182 (98%)	3 (2%)	62	88
9	I	172/173 (99%)	170 (99%)	2 (1%)	71	92
9	W	172/173 (99%)	170 (99%)	2 (1%)	71	92
10	J	173/175 (99%)	170 (98%)	3 (2%)	60	87
10	X	173/175 (99%)	170 (98%)	3 (2%)	60	87
11	K	165/165 (100%)	153 (93%)	12 (7%)	14	38
11	Y	165/165 (100%)	152 (92%)	13 (8%)	12	34
12	L	186/186 (100%)	179 (96%)	7 (4%)	33	67
12	Z	186/186 (100%)	182 (98%)	4 (2%)	52	83
13	M	199/208 (96%)	193 (97%)	6 (3%)	41	75
13	a	200/208 (96%)	194 (97%)	6 (3%)	41	75

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	N	162/162 (100%)	156 (96%)	6 (4%)	34	68
14	b	162/162 (100%)	156 (96%)	6 (4%)	34	68
All	All	5315/5534 (96%)	5151 (97%)	164 (3%)	40	74

All (164) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	122	THR
1	A	157	PHE
1	A	250	LEU
2	B	55	LEU
2	B	113	ARG
2	B	191	LEU
2	B	238	LEU
3	C	4	ARG
3	C	38	ASN
3	C	51	LYS
3	C	147	GLN
3	C	160	GLN
3	C	169	VAL
3	C	180	LYS
3	C	206	LYS
3	C	240	GLU
4	D	99	ILE
4	D	125	LEU
4	D	143	ASP
4	D	176	LEU
4	D	193	LEU
4	D	214	ILE
4	D	235	LEU
4	D	236	LYS
4	D	242	GLU
5	E	9	THR
5	E	29	LYS
5	E	71	LEU
5	E	184	ASN
5	E	188	LEU
5	E	202	ASP
6	F	117	GLN
6	F	123	ASN
6	F	139	LYS

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Mol	Chain	Res	Type
6	F	171	GLU
6	F	181	GLU
6	F	214	TRP
6	F	240	GLN
7	G	115	LEU
7	G	122	ARG
7	G	125	MET
7	G	208	GLU
7	G	235	ARG
7	G	236	LEU
8	H	30	ASN
8	H	68	LEU
8	H	196	ARG
9	I	37	ASN
9	I	171	LEU
10	J	3	ILE
10	J	23	ARG
10	J	99	GLN
11	K	4	LEU
11	K	12	VAL
11	K	21	THR
11	K	29	GLN
11	K	38	ASN
11	K	57	ARG
11	K	62	GLN
11	K	71	LYS
11	K	83	LEU
11	K	86	MET
11	K	117	GLU
11	K	128	VAL
12	L	23	LEU
12	L	49	ASN
12	L	100	ARG
12	L	101	ARG
12	L	130	SER
12	L	132	GLN
12	L	150	LEU
13	M	2	GLN
13	M	48	ASN
13	M	70	LEU
13	M	104	ARG
13	M	161	ARG

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Mol	Chain	Res	Type
13	M	187	ARG
14	N	9	LYS
14	N	36	ARG
14	N	39	ASP
14	N	83	LYS
14	N	104	ASP
14	N	178	LEU
1	O	122	THR
1	O	157	PHE
1	O	250	LEU
2	P	55	LEU
2	P	113	ARG
2	P	191	LEU
2	P	238	LEU
3	Q	4	ARG
3	Q	38	ASN
3	Q	51	LYS
3	Q	147	GLN
3	Q	160	GLN
3	Q	169	VAL
3	Q	180	LYS
3	Q	206	LYS
3	Q	240	GLU
4	R	99	ILE
4	R	125	LEU
4	R	143	ASP
4	R	176	LEU
4	R	193	LEU
4	R	214	ILE
4	R	235	LEU
4	R	236	LYS
4	R	242	GLU
5	S	9	THR
5	S	29	LYS
5	S	71	LEU
5	S	184	ASN
5	S	188	LEU
5	S	202	ASP
6	T	117	GLN
6	T	123	ASN
6	T	139	LYS
6	T	171	GLU

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Mol	Chain	Res	Type
6	T	181	GLU
6	T	214	TRP
6	T	240	GLN
7	U	115	LEU
7	U	122	ARG
7	U	125	MET
7	U	208	GLU
7	U	235	ARG
7	U	236	LEU
8	V	30	ASN
8	V	68	LEU
8	V	196	ARG
9	W	37	ASN
9	W	171	LEU
10	X	3	ILE
10	X	23	ARG
10	X	99	GLN
11	Y	4	LEU
11	Y	12	VAL
11	Y	21	THR
11	Y	29	GLN
11	Y	38	ASN
11	Y	57	ARG
11	Y	61	ARG
11	Y	62	GLN
11	Y	71	LYS
11	Y	83	LEU
11	Y	86	MET
11	Y	117	GLU
11	Y	128	VAL
12	Z	23	LEU
12	Z	49	ASN
12	Z	130	SER
12	Z	150	LEU
13	a	2	GLN
13	a	48	ASN
13	a	70	LEU
13	a	104	ARG
13	a	161	ARG
13	a	187	ARG
14	b	9	LYS
14	b	36	ARG

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Mol	Chain	Res	Type
14	b	39	ASP
14	b	83	LYS
14	b	104	ASP
14	b	178	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (90) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	94	HIS
2	B	58	GLN
2	B	119	GLN
2	B	123	GLN
3	C	17	GLN
3	C	147	GLN
3	C	160	GLN
4	D	15	GLN
4	D	91	HIS
4	D	146	GLN
4	D	225	ASN
5	E	68	HIS
5	E	92	ASN
5	E	99	ASN
5	E	116	GLN
5	E	118	ASN
5	E	120	GLN
5	E	151	ASN
5	E	184	ASN
6	F	19	GLN
6	F	86	ASN
6	F	117	GLN
6	F	123	ASN
6	F	191	GLN
7	G	83	ASN
7	G	114	ASN
7	G	117	GLN
7	G	121	GLN
7	G	166	GLN
8	H	35	HIS
9	I	37	ASN
10	J	55	GLN
11	K	85	ASN
11	K	175	ASN

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Mol	Chain	Res	Type
11	K	207	ASN
12	L	3	ASN
12	L	49	ASN
12	L	70	ASN
12	L	79	HIS
12	L	158	ASN
13	M	48	ASN
13	M	102	GLN
13	M	179	ASN
13	M	194	ASN
13	M	213	GLN
14	N	161	GLN
1	O	94	HIS
2	P	20	GLN
2	P	58	GLN
2	P	119	GLN
2	P	123	GLN
3	Q	147	GLN
3	Q	160	GLN
4	R	91	HIS
4	R	146	GLN
4	R	225	ASN
5	S	68	HIS
5	S	99	ASN
5	S	116	GLN
5	S	118	ASN
5	S	120	GLN
5	S	151	ASN
5	S	184	ASN
6	T	19	GLN
6	T	86	ASN
6	T	117	GLN
6	T	123	ASN
6	T	191	GLN
7	U	83	ASN
7	U	114	ASN
7	U	117	GLN
7	U	121	GLN
7	U	166	GLN
8	V	35	HIS
9	W	37	ASN
10	X	55	GLN

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Mol	Chain	Res	Type
11	Y	85	ASN
11	Y	175	ASN
11	Y	207	ASN
12	Z	3	ASN
12	Z	49	ASN
12	Z	79	HIS
12	Z	94	GLN
12	Z	158	ASN
13	a	48	ASN
13	a	102	GLN
13	a	179	ASN
13	a	194	ASN
13	a	213	GLN
14	b	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)

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 16 ligands modelled in this entry, 16 are monoatomic - leaving 0 for Mogul analysis.

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.

No monomer is involved in short contacts.

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 (i)

6.1 Protein, DNA and RNA chains (i)

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	250/250 (100%)	-0.46	6 (2%)	59	49	33, 50, 89, 127	0
1	O	250/250 (100%)	-0.42	8 (3%)	47	37	37, 54, 100, 136	0
2	B	244/258 (94%)	-0.40	7 (2%)	51	41	38, 55, 99, 156	0
2	P	244/258 (94%)	-0.40	7 (2%)	51	41	41, 58, 101, 154	0
3	C	240/254 (94%)	-0.22	11 (4%)	32	22	36, 64, 130, 167	0
3	Q	240/254 (94%)	-0.16	12 (5%)	28	19	37, 68, 138, 181	0
4	D	235/260 (90%)	-0.44	1 (0%)	92	91	42, 60, 90, 129	0
4	R	235/260 (90%)	-0.34	5 (2%)	63	54	49, 67, 106, 134	0
5	E	231/234 (98%)	-0.42	1 (0%)	92	91	41, 60, 99, 139	0
5	S	231/234 (98%)	-0.38	3 (1%)	77	72	45, 64, 101, 134	0
6	F	243/288 (84%)	-0.52	5 (2%)	63	54	36, 56, 102, 128	0
6	T	243/288 (84%)	-0.45	4 (1%)	72	66	37, 62, 114, 143	0
7	G	241/252 (95%)	-0.53	4 (1%)	70	63	35, 53, 93, 149	0
7	U	241/252 (95%)	-0.50	3 (1%)	79	73	37, 53, 87, 125	0
8	H	226/232 (97%)	-0.52	5 (2%)	62	52	34, 49, 84, 149	0
8	V	226/232 (97%)	-0.49	5 (2%)	62	52	35, 50, 82, 164	0
9	I	204/205 (99%)	-0.71	1 (0%)	91	88	32, 47, 75, 97	0
9	W	204/205 (99%)	-0.70	1 (0%)	91	88	29, 48, 74, 100	0
10	J	195/198 (98%)	-0.45	3 (1%)	73	68	36, 55, 86, 131	0
10	X	195/198 (98%)	-0.47	3 (1%)	73	68	38, 57, 89, 136	0
11	K	211/211 (100%)	-0.46	1 (0%)	91	88	36, 54, 82, 112	0
11	Y	211/211 (100%)	-0.41	2 (0%)	84	80	37, 56, 88, 112	0
12	L	222/222 (100%)	-0.43	3 (1%)	75	70	41, 55, 99, 128	0
12	Z	222/222 (100%)	-0.41	5 (2%)	60	51	38, 57, 99, 130	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	M	233/246 (94%)	-0.65	0 100 100	33, 50, 72, 90	0
13	a	233/246 (94%)	-0.61	1 (0%) 92 91	33, 52, 75, 92	0
14	N	196/196 (100%)	-0.63	0 100 100	34, 46, 77, 102	0
14	b	196/196 (100%)	-0.67	2 (1%) 82 77	33, 46, 76, 106	0
All	All	6342/6612 (95%)	-0.47	109 (1%) 70 63	29, 55, 98, 181	0

All (109) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
10	J	1	MET	7.3
9	W	1	SER	6.7
10	X	1	MET	5.5
2	B	221	ASP	5.3
3	C	206	LYS	4.9
3	Q	206	LYS	4.9
1	O	1	MET	4.8
8	V	224	GLN	4.8
5	E	202	ASP	4.6
3	Q	240	GLU	4.4
2	P	51	VAL	4.3
9	I	1	SER	4.3
2	P	219	ALA	4.2
3	Q	238	LYS	4.0
3	Q	237	GLU	4.0
1	A	1	MET	3.9
2	B	218	GLY	3.9
8	V	145	ASP	3.7
8	V	222	ASP	3.7
3	C	238	LYS	3.7
3	Q	239	GLN	3.7
2	P	221	ASP	3.6
3	Q	202	GLN	3.6
8	H	226	GLU	3.6
1	O	2	THR	3.5
3	C	239	GLN	3.5
10	J	194	ASP	3.4
8	V	226	GLU	3.4
12	L	174	TYR	3.3
6	F	181	GLU	3.2
11	K	146	ASP	3.1
5	S	202	ASP	3.0

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Mol	Chain	Res	Type	RSRZ
2	B	220	ASN	3.0
12	Z	1	GLN	3.0
5	S	3	ASN	3.0
8	H	224	GLN	3.0
12	Z	174	TYR	3.0
7	U	2	GLY	3.0
10	X	193	ASP	2.9
2	B	51	VAL	2.9
6	T	181	GLU	2.9
3	C	50	LEU	2.8
11	Y	182	ASP	2.8
1	A	249	ALA	2.8
1	O	248	GLU	2.8
6	T	244	ASN	2.8
6	F	202	ASP	2.8
8	H	222	ASP	2.8
10	X	194	ASP	2.8
12	L	1	GLN	2.8
2	B	217	LYS	2.7
2	P	218	GLY	2.7
4	R	241	ALA	2.7
3	C	205	ALA	2.7
3	C	202	GLN	2.7
13	a	1	THR	2.7
7	G	241	GLU	2.6
10	J	193	ASP	2.6
4	R	217	GLN	2.6
2	B	219	ALA	2.6
2	P	59	ASP	2.5
4	R	230	GLU	2.5
12	Z	167	LYS	2.5
6	F	205	GLU	2.5
3	Q	50	LEU	2.5
3	C	203	THR	2.4
1	O	231	LYS	2.4
8	H	221	CYS	2.4
2	P	220	ASN	2.4
3	C	216	ASP	2.4
11	Y	146	ASP	2.4
12	Z	210	ASP	2.4
3	C	236	GLN	2.4
2	P	203	SER	2.4

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Mol	Chain	Res	Type	RSRZ
14	b	195	GLN	2.3
4	R	242	GLU	2.3
8	V	9	ASN	2.3
3	Q	181	GLU	2.3
4	R	203	LYS	2.3
7	U	181	LYS	2.3
3	C	139	ARG	2.3
1	O	249	ALA	2.3
3	Q	236	GLN	2.3
1	A	2	THR	2.2
6	F	244	ASN	2.2
5	S	203	GLU	2.2
12	L	166	GLY	2.2
1	A	201	GLU	2.2
3	Q	225	GLU	2.2
3	Q	49	THR	2.2
1	O	201	GLU	2.2
3	Q	204	GLY	2.2
1	O	53	SER	2.2
3	C	49	THR	2.2
1	O	250	LEU	2.2
14	b	105	LYS	2.1
1	A	248	GLU	2.1
8	H	225	GLU	2.1
6	F	2	THR	2.1
12	Z	172	LEU	2.1
7	G	242	GLN	2.1
2	B	182	ASP	2.1
7	G	2	GLY	2.1
7	G	188	GLU	2.1
4	D	242	GLU	2.0
6	T	180	PRO	2.0
7	U	242	GLN	2.0
6	T	205	GLU	2.0
1	A	228	PRO	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
16	MG	M	301	1/1	0.76	0.48	68,68,68,68	0
16	MG	K	302	1/1	0.81	0.37	59,59,59,59	0
16	MG	N	201	1/1	0.87	0.22	59,59,59,59	0
16	MG	J	201	1/1	0.92	0.21	60,60,60,60	0
16	MG	Z	301	1/1	0.93	0.19	78,78,78,78	0
16	MG	H	301	1/1	0.94	0.14	56,56,56,56	0
16	MG	b	201	1/1	0.94	0.14	54,54,54,54	0
15	CL	b	202	1/1	0.96	0.22	53,53,53,53	0
16	MG	I	301	1/1	0.96	0.16	45,45,45,45	0
16	MG	I	302	1/1	0.96	0.07	53,53,53,53	0
16	MG	G	301	1/1	0.97	0.05	46,46,46,46	0
15	CL	U	301	1/1	0.98	0.17	41,41,41,41	0
15	CL	E	301	1/1	0.98	0.03	58,58,58,58	0
15	CL	G	302	1/1	0.99	0.17	44,44,44,44	0
16	MG	L	301	1/1	0.99	0.05	60,60,60,60	0
16	MG	K	301	1/1	0.99	0.04	52,52,52,52	0

6.5 Other polymers (i)

There are no such residues in this entry.