wwPDB X-ray Structure Validation Summary Report (i)

Jun 13, 2024 – 01:56 AM EDT

PDB ID	:	3WXR
Title	:	Yeast 20S proteasome with a mutation of alpha7 subunit
Authors	:	Yashiroda, H.; Toda, Y.; Otsu, S.; Takagi, K.; Mizushima, T.; Murata, S.
Deposited on	:	2014-08-06
Resolution	:	3.15 Å(reported)

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

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

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

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

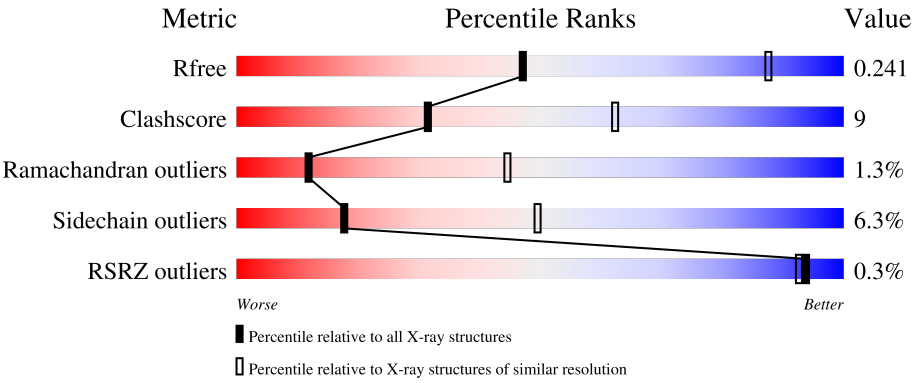
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.20.1
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 3.15 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.



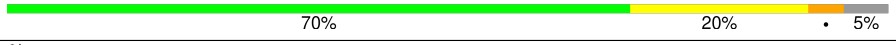
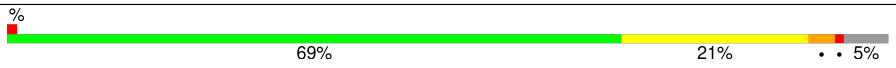
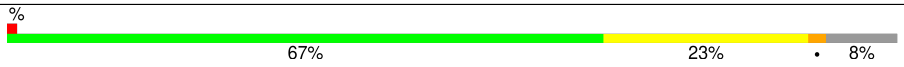
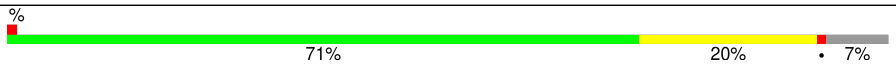
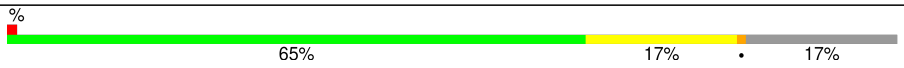
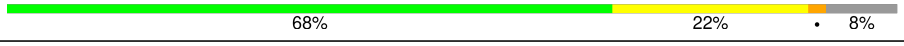
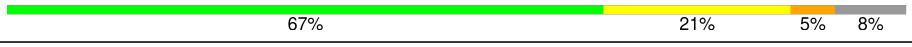
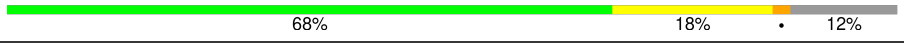
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1665 (3.20-3.12)
Clashscore	141614	1804 (3.20-3.12)
Ramachandran outliers	138981	1770 (3.20-3.12)
Sidechain outliers	138945	1769 (3.20-3.12)
RSRZ outliers	127900	1616 (3.20-3.12)

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	252	% 77% 16%
1	O	252	75% 18%
2	B	250	78% 20%
2	P	250	80% 18%
3	C	258	66% 24% 6%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	Q	258	
4	D	254	
4	R	254	
5	E	260	
5	S	260	
6	F	234	
6	T	234	
7	G	277	
7	U	277	
8	H	215	
8	V	215	
9	I	261	
9	W	261	
10	J	205	
10	X	205	
11	K	238	
11	Y	238	
12	L	287	
12	Z	287	
13	1	241	
13	M	241	
14	2	266	
14	N	266	

2 Entry composition (i)

There are 14 unique types of molecules in this entry. The entry contains 49360 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-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	243	Total	C	N	O	S	0	0	0
			1921	1221	322	370	8			
1	O	243	Total	C	N	O	S	0	0	0
			1920	1221	322	369	8			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	249	Total	C	N	O	S	0	0	0
			1907	1214	314	376	3			
2	P	249	Total	C	N	O	S	0	0	0
			1907	1214	314	376	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	242	Total	C	N	O	S	0	0	0
			1895	1196	319	377	3			
3	Q	244	Total	C	N	O	S	0	0	0
			1904	1201	321	379	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
			1890	1181	331	374	4			
4	R	241	Total	C	N	O	S	0	0	0
			1890	1181	331	374	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	239	Total	C	N	O	S	0	0	0
			1842	1152	311	372	7			
5	S	238	Total	C	N	O	S	0	0	0
			1842	1152	310	373	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
			1784	1120	311	349	4			
6	T	232	Total	C	N	O	S	0	0	0
			1784	1120	311	349	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	237	Total	C	N	O	S	0	0	0
			1847	1176	322	344	5			
7	U	237	Total	C	N	O	S	0	0	0
			1847	1176	322	344	5			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	11	MET	-	expression tag	UNP P21242
U	11	MET	-	expression tag	UNP P21242

- 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	199	Total	C	N	O	S	0	0	0
			1528	965	253	303	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			
10	X	204	Total	C	N	O	S	0	0	0
			1581	1010	258	305	8			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	197	Total	C	N	O	S	0	0	0
			1576	1000	268	303	5			
11	Y	198	Total	C	N	O	S	0	0	0
			1584	1005	269	304	6			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	198	GLY	-	expression tag	UNP P22141
K	199	SER	-	expression tag	UNP P22141
K	200	GLY	-	expression tag	UNP P22141
K	201	SER	-	expression tag	UNP P22141
K	202	LEU	-	expression tag	UNP P22141
K	203	GLU	-	expression tag	UNP P22141
K	204	VAL	-	expression tag	UNP P22141
K	205	LEU	-	expression tag	UNP P22141
K	206	PHE	-	expression tag	UNP P22141
K	207	GLN	-	expression tag	UNP P22141
K	208	GLY	-	expression tag	UNP P22141
K	209	PRO	-	expression tag	UNP P22141
K	210	GLY	-	expression tag	UNP P22141
K	211	SER	-	expression tag	UNP P22141
K	212	GLY	-	expression tag	UNP P22141
K	213	SER	-	expression tag	UNP P22141
K	214	THR	-	expression tag	UNP P22141
K	215	MET	-	expression tag	UNP P22141
K	216	ASP	-	expression tag	UNP P22141
K	217	TYR	-	expression tag	UNP P22141
K	218	LYS	-	expression tag	UNP P22141
K	219	ASP	-	expression tag	UNP P22141
K	220	HIS	-	expression tag	UNP P22141
K	221	ASP	-	expression tag	UNP P22141
K	222	GLY	-	expression tag	UNP P22141

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
K	223	ASP	-	expression tag	UNP P22141
K	224	TYR	-	expression tag	UNP P22141
K	225	LYS	-	expression tag	UNP P22141
K	226	ASP	-	expression tag	UNP P22141
K	227	HIS	-	expression tag	UNP P22141
K	228	ASP	-	expression tag	UNP P22141
K	229	ILE	-	expression tag	UNP P22141
K	230	ASP	-	expression tag	UNP P22141
K	231	TYR	-	expression tag	UNP P22141
K	232	LYS	-	expression tag	UNP P22141
K	233	ASP	-	expression tag	UNP P22141
K	234	ASP	-	expression tag	UNP P22141
K	235	ASP	-	expression tag	UNP P22141
K	236	ASP	-	expression tag	UNP P22141
K	237	LYS	-	expression tag	UNP P22141
Y	198	GLY	-	expression tag	UNP P22141
Y	199	SER	-	expression tag	UNP P22141
Y	200	GLY	-	expression tag	UNP P22141
Y	201	SER	-	expression tag	UNP P22141
Y	202	LEU	-	expression tag	UNP P22141
Y	203	GLU	-	expression tag	UNP P22141
Y	204	VAL	-	expression tag	UNP P22141
Y	205	LEU	-	expression tag	UNP P22141
Y	206	PHE	-	expression tag	UNP P22141
Y	207	GLN	-	expression tag	UNP P22141
Y	208	GLY	-	expression tag	UNP P22141
Y	209	PRO	-	expression tag	UNP P22141
Y	210	GLY	-	expression tag	UNP P22141
Y	211	SER	-	expression tag	UNP P22141
Y	212	GLY	-	expression tag	UNP P22141
Y	213	SER	-	expression tag	UNP P22141
Y	214	THR	-	expression tag	UNP P22141
Y	215	MET	-	expression tag	UNP P22141
Y	216	ASP	-	expression tag	UNP P22141
Y	217	TYR	-	expression tag	UNP P22141
Y	218	LYS	-	expression tag	UNP P22141
Y	219	ASP	-	expression tag	UNP P22141
Y	220	HIS	-	expression tag	UNP P22141
Y	221	ASP	-	expression tag	UNP P22141
Y	222	GLY	-	expression tag	UNP P22141
Y	223	ASP	-	expression tag	UNP P22141
Y	224	TYR	-	expression tag	UNP P22141

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
Y	225	LYS	-	expression tag	UNP P22141
Y	226	ASP	-	expression tag	UNP P22141
Y	227	HIS	-	expression tag	UNP P22141
Y	228	ASP	-	expression tag	UNP P22141
Y	229	ILE	-	expression tag	UNP P22141
Y	230	ASP	-	expression tag	UNP P22141
Y	231	TYR	-	expression tag	UNP P22141
Y	232	LYS	-	expression tag	UNP P22141
Y	233	ASP	-	expression tag	UNP P22141
Y	234	ASP	-	expression tag	UNP P22141
Y	235	ASP	-	expression tag	UNP P22141
Y	236	ASP	-	expression tag	UNP P22141
Y	237	LYS	-	expression tag	UNP P22141

- 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
			1644	1045	280	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
			1757	1115	303	335	4			
13	1	222	Total	C	N	O	S	0	0	0
			1757	1115	303	335	4			

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

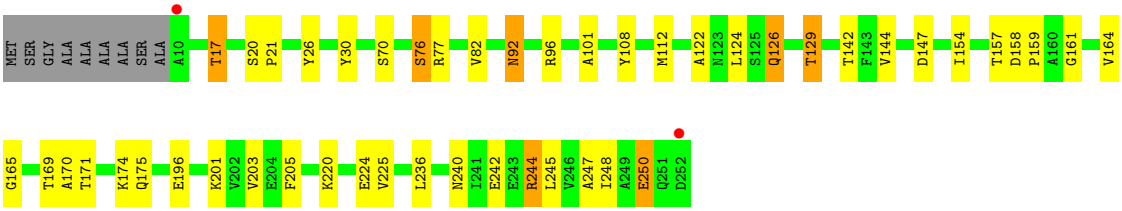
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	N	233	Total	C	N	O	S	0	0	0
			1824	1154	312	351	7			
14	2	233	Total	C	N	O	S	0	0	0
			1824	1154	312	351	7			

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.

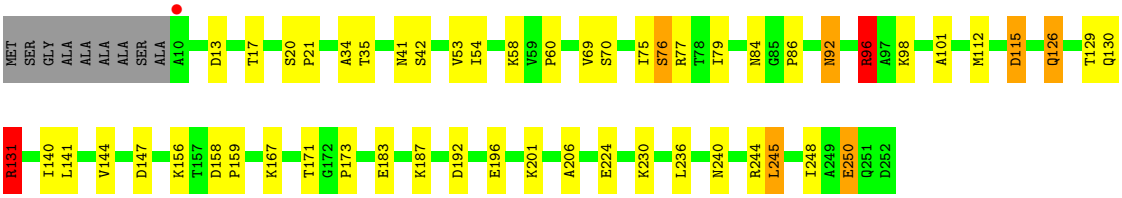
• Molecule 1: Proteasome subunit alpha type-1

Chain A:



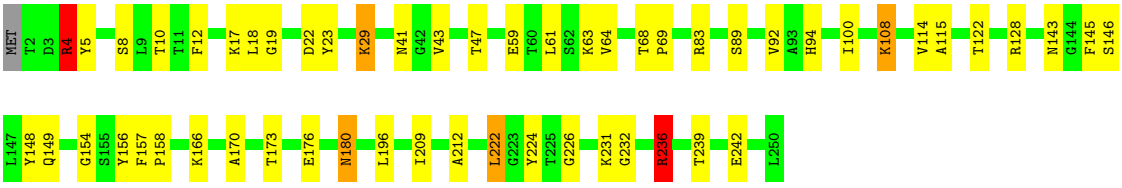
• Molecule 1: Proteasome subunit alpha type-1

Chain O:



• Molecule 2: Proteasome subunit alpha type-2

Chain B:

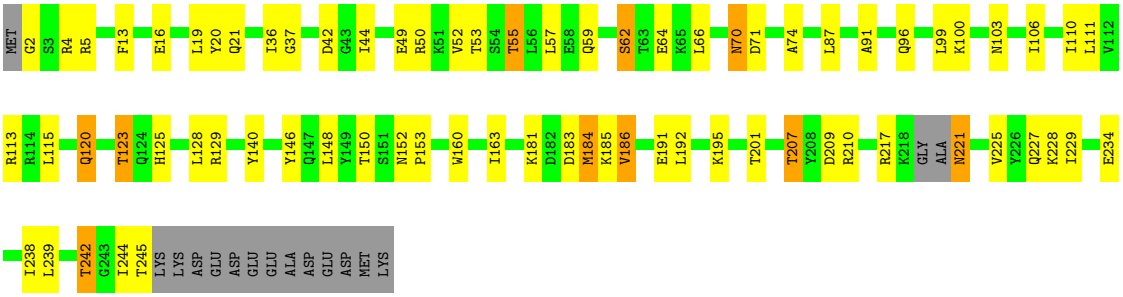


• Molecule 2: Proteasome subunit alpha type-2

Chain P:

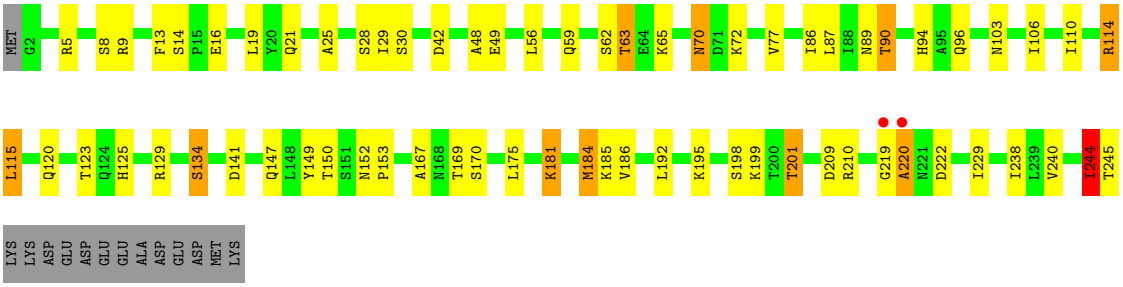
• Molecule 3: Proteasome subunit alpha type-3

Chain C:



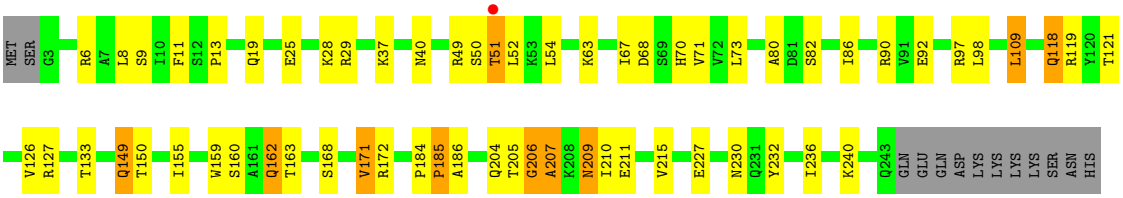
• Molecule 3: Proteasome subunit alpha type-3

Chain Q:



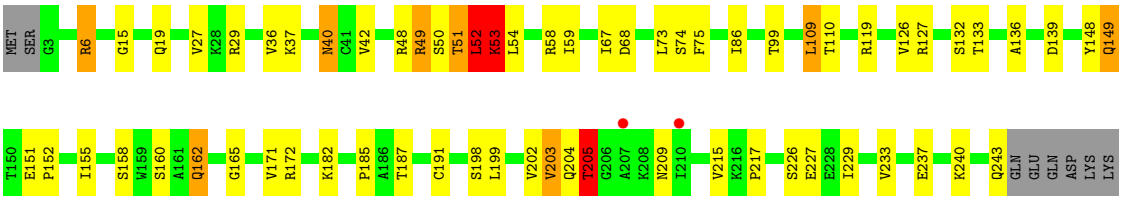
• Molecule 4: Proteasome subunit alpha type-4

Chain D:



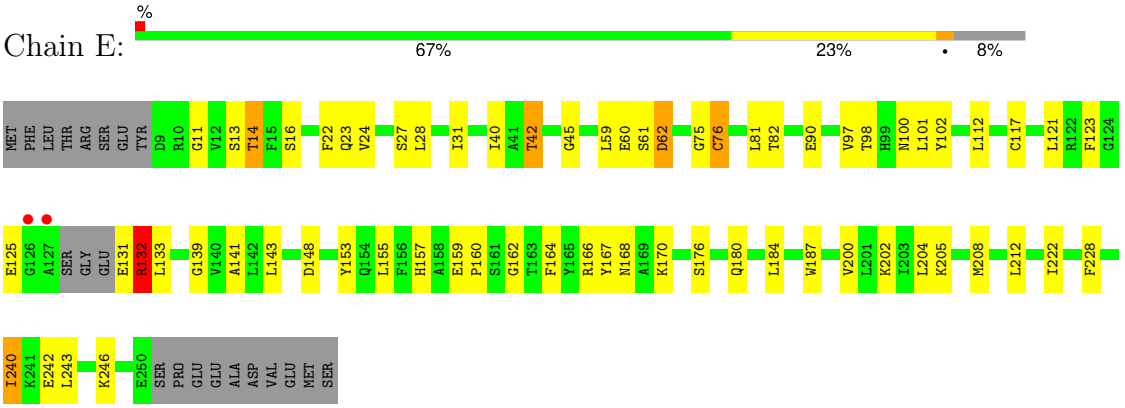
• Molecule 4: Proteasome subunit alpha type-4

Chain R:



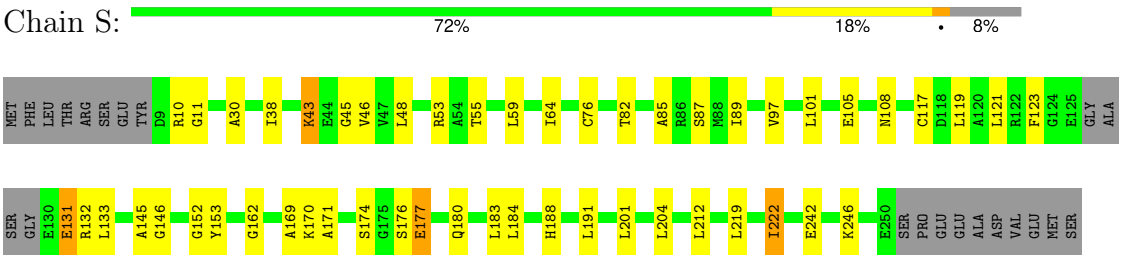
• Molecule 5: Proteasome subunit alpha type-5

Chain E:



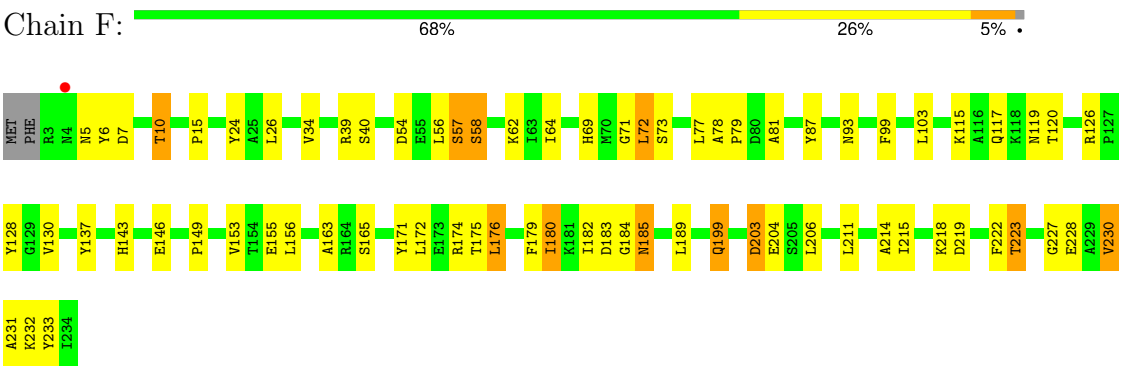
• Molecule 5: Proteasome subunit alpha type-5

Chain S:



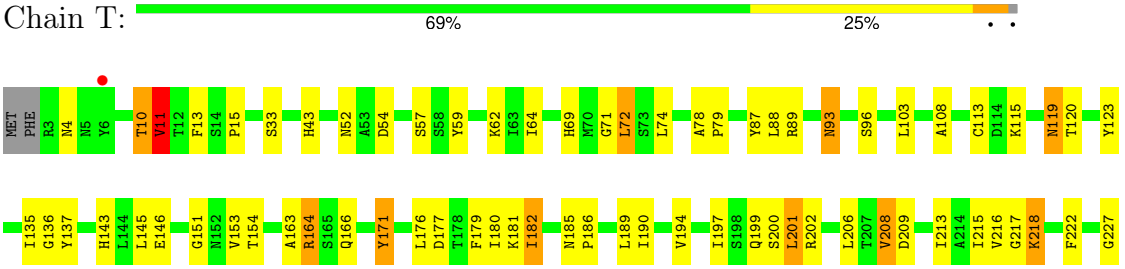
• Molecule 6: Proteasome subunit alpha type-6

Chain F:



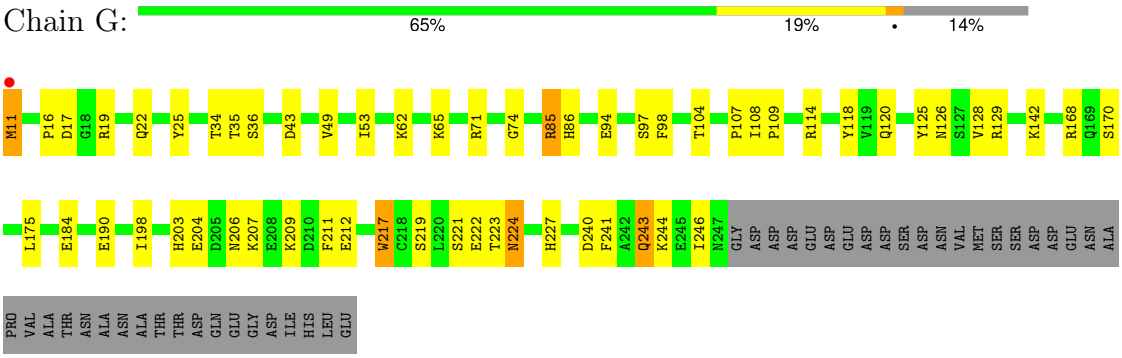
• Molecule 6: Proteasome subunit alpha type-6

Chain T:



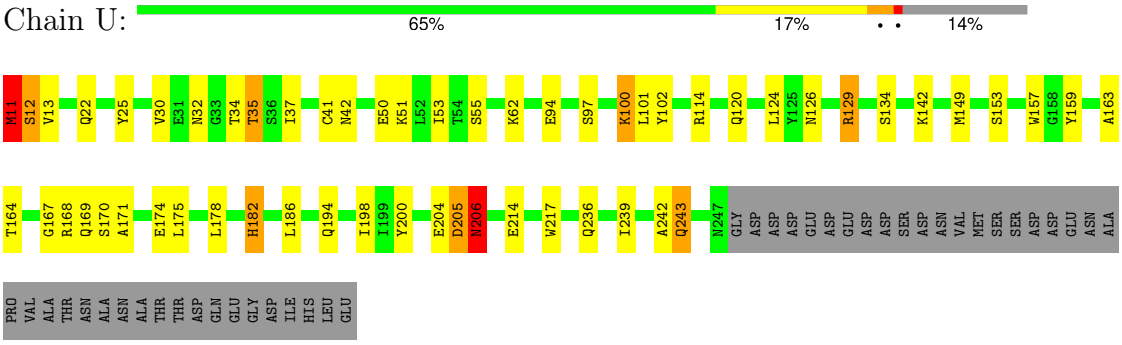
• Molecule 7: Probable proteasome subunit alpha type-7

Chain G:



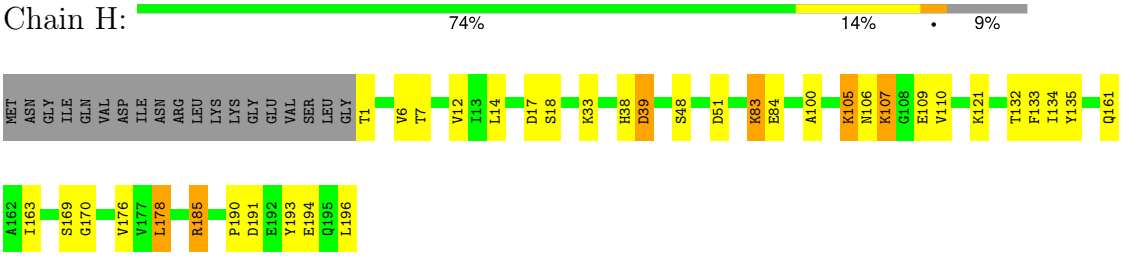
• Molecule 7: Probable proteasome subunit alpha type-7

Chain U:



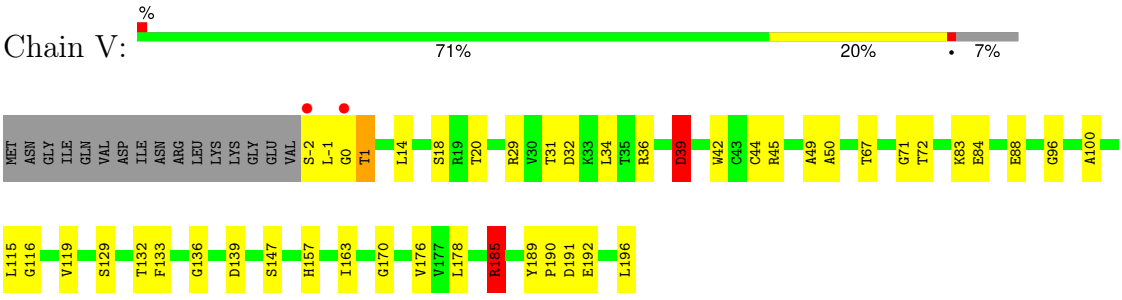
• Molecule 8: Proteasome subunit beta type-1

Chain H:



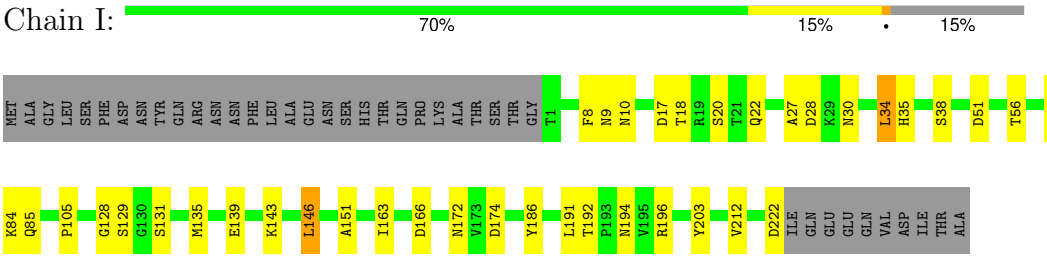
• Molecule 8: Proteasome subunit beta type-1

Chain V:



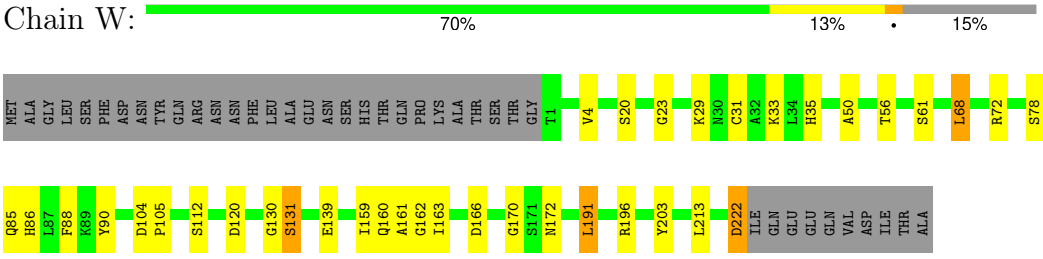
• Molecule 9: Proteasome subunit beta type-2

Chain I:



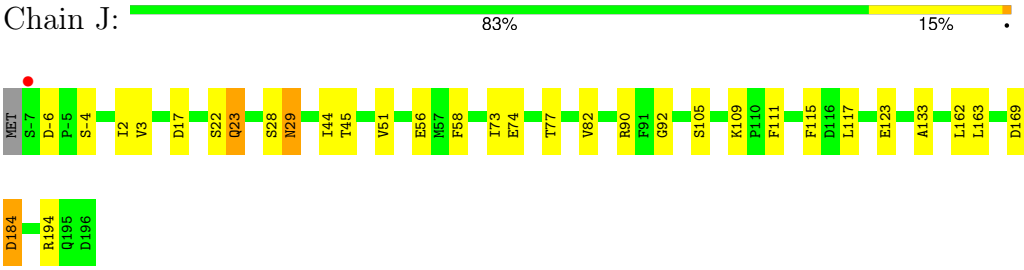
• Molecule 9: Proteasome subunit beta type-2

Chain W:



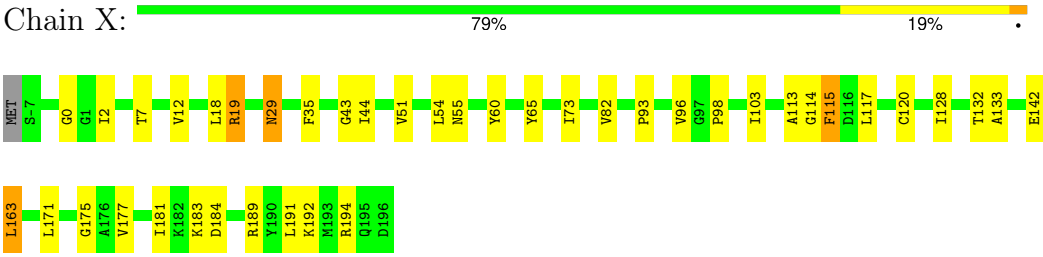
• Molecule 10: Proteasome subunit beta type-3

Chain J:



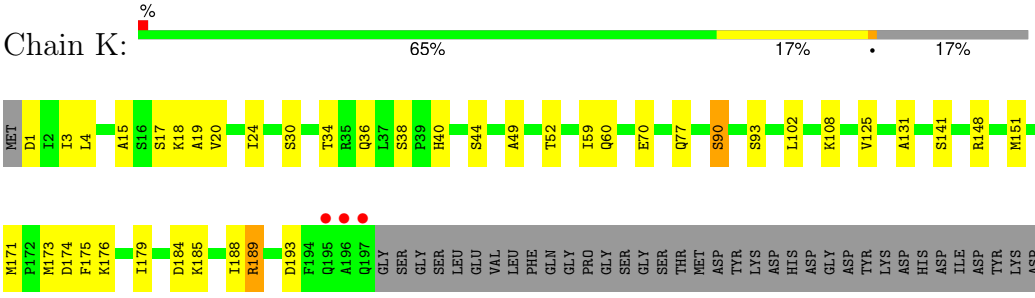
• Molecule 10: Proteasome subunit beta type-3

Chain X:



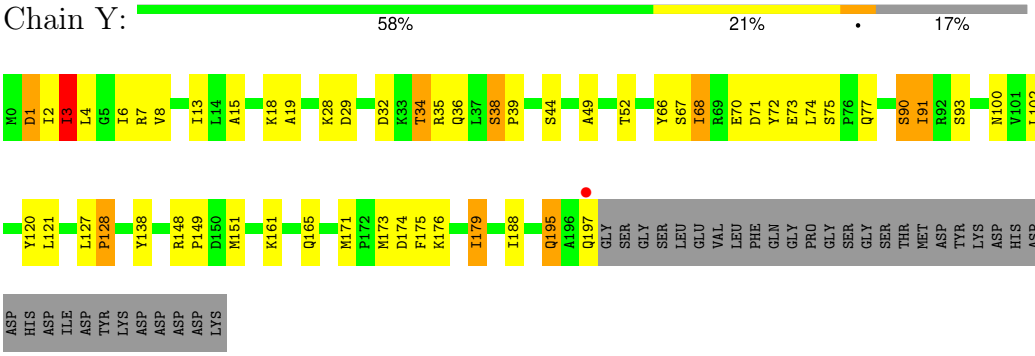
• Molecule 11: Proteasome subunit beta type-4

Chain K:



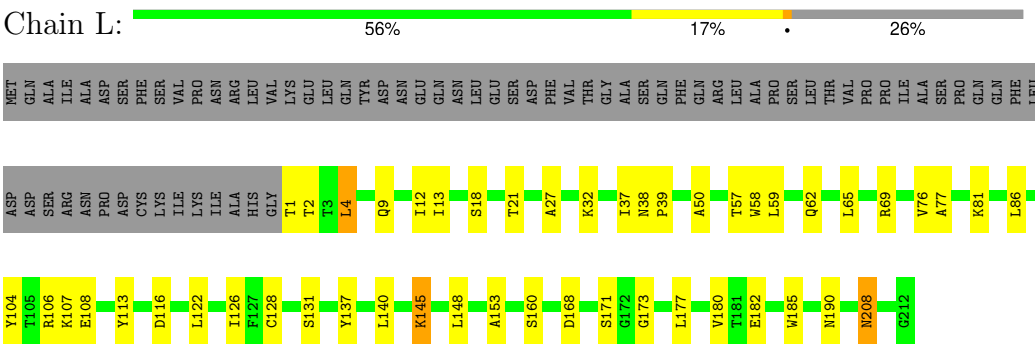
• Molecule 11: Proteasome subunit beta type-4

Chain Y:



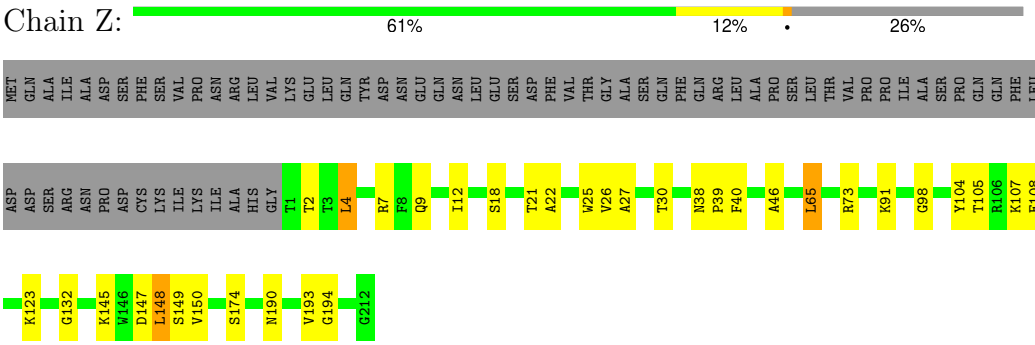
• Molecule 12: Proteasome subunit beta type-5

Chain L:



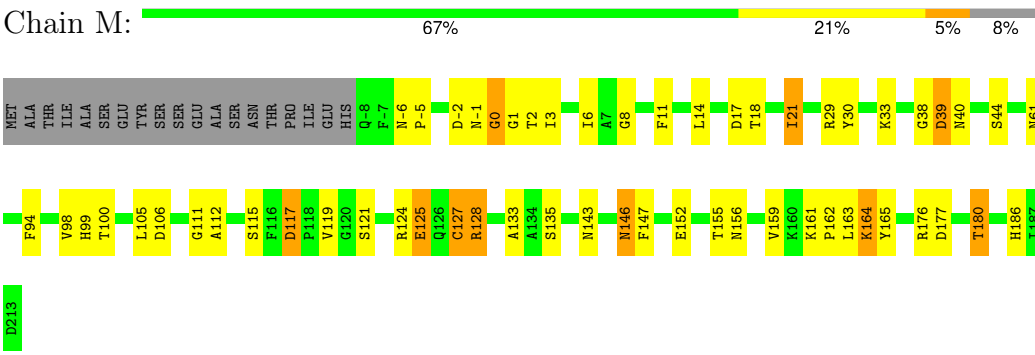
• Molecule 12: Proteasome subunit beta type-5

Chain Z:



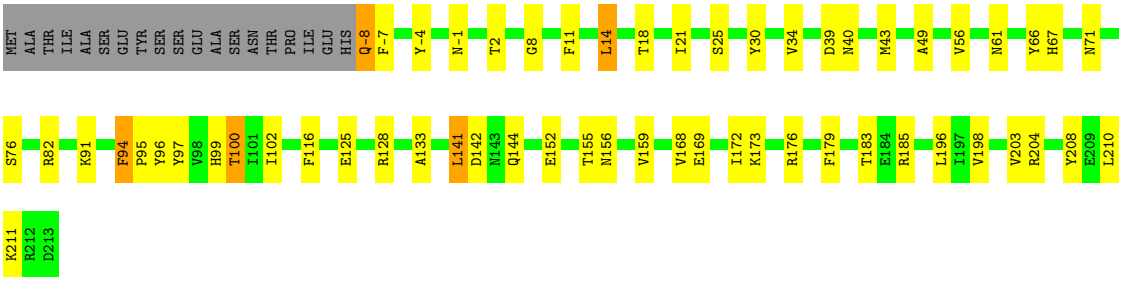
• Molecule 13: Proteasome subunit beta type-6

Chain M:



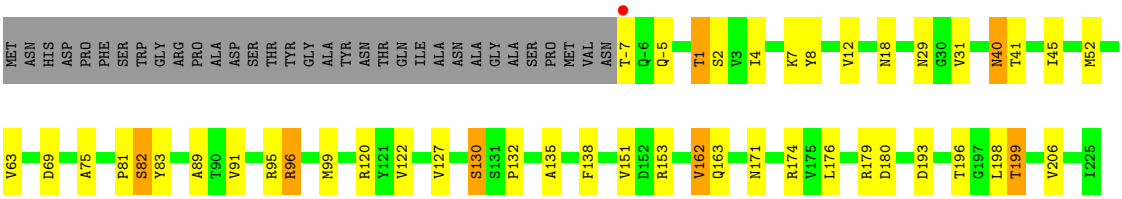
• Molecule 13: Proteasome subunit beta type-6

Chain 1:



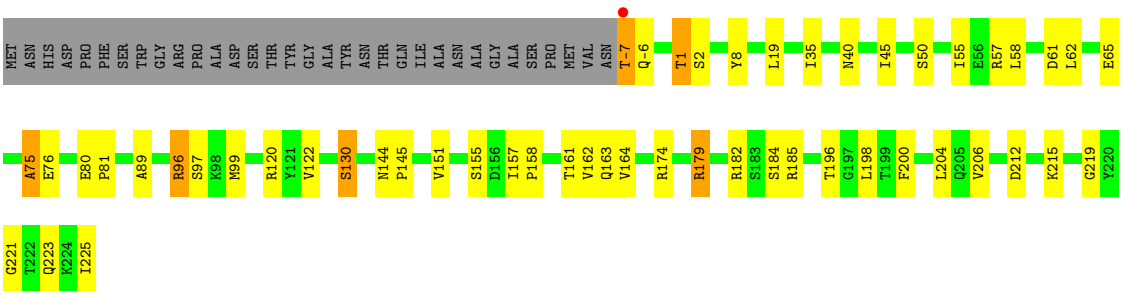
• Molecule 14: Proteasome subunit beta type-7

Chain N:



• Molecule 14: Proteasome subunit beta type-7

Chain 2:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	137.25Å 298.62Å 145.40Å 90.00° 113.13° 90.00°	Depositor
Resolution (Å)	48.20 – 3.15 48.20 – 3.15	Depositor EDS
% Data completeness (in resolution range)	86.6 (48.20-3.15) 86.7 (48.20-3.15)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.39 (at 3.12Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.174 , 0.242 0.176 , 0.241	Depositor DCC
R_{free} test set	8012 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	52.0	Xtriage
Anisotropy	0.080	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 25.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	49360	wwPDB-VP
Average B, all atoms (Å^2)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.08% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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	0.59	0/1959	0.87	0/2652
1	O	0.57	0/1958	0.88	2/2652 (0.1%)
2	B	0.57	0/1944	0.85	2/2632 (0.1%)
2	P	0.52	0/1944	0.80	0/2632
3	C	0.55	0/1924	0.87	1/2603 (0.0%)
3	Q	0.56	0/1934	0.85	0/2618
4	D	0.53	0/1919	0.88	1/2598 (0.0%)
4	R	0.55	0/1919	0.88	3/2598 (0.1%)
5	E	0.57	0/1866	0.89	1/2513 (0.0%)
5	S	0.53	0/1866	0.85	0/2513
6	F	0.53	0/1811	0.83	0/2447
6	T	0.52	0/1811	0.85	0/2447
7	G	0.55	0/1886	0.81	0/2545
7	U	0.55	0/1886	0.84	1/2545 (0.0%)
8	H	0.59	0/1541	0.88	0/2087
8	V	0.61	0/1557	0.90	3/2108 (0.1%)
9	I	0.58	0/1715	0.87	0/2326
9	W	0.54	0/1715	0.84	1/2326 (0.0%)
10	J	0.59	0/1611	0.85	0/2174
10	X	0.59	0/1611	0.83	0/2174
11	K	0.60	0/1604	0.91	0/2163
11	Y	0.57	0/1612	0.90	1/2173 (0.0%)
12	L	0.60	0/1681	0.86	0/2274
12	Z	0.60	0/1681	0.86	0/2274
13	1	0.57	0/1795	0.88	0/2420
13	M	0.61	0/1795	0.91	1/2420 (0.0%)
14	2	0.61	0/1855	0.90	0/2514
14	N	0.58	0/1855	0.89	1/2514 (0.0%)
All	All	0.57	0/50255	0.87	18/67942 (0.0%)

There are no bond length outliers.

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	71	ASP	CB-CG-OD1	-7.67	111.39	118.30
1	O	131	ARG	NE-CZ-NH1	7.58	124.09	120.30
2	B	236	ARG	NE-CZ-NH2	7.41	124.00	120.30
7	U	11	MET	CG-SD-CE	7.20	111.72	100.20
4	R	52	LEU	CA-CB-CG	7.18	131.82	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1921	0	1910	32	0
1	O	1920	0	1910	42	0
2	B	1907	0	1917	46	0
2	P	1907	0	1917	35	0
3	C	1895	0	1892	50	0
3	Q	1904	0	1901	42	0
4	D	1890	0	1900	42	0
4	R	1890	0	1900	42	0
5	E	1842	0	1821	45	0
5	S	1842	0	1819	26	0
6	F	1784	0	1788	49	0
6	T	1784	0	1788	46	0
7	G	1847	0	1847	25	0
7	U	1847	0	1847	43	0
8	H	1512	0	1481	26	0
8	V	1528	0	1495	28	0
9	I	1684	0	1688	25	0
9	W	1684	0	1688	28	0
10	J	1581	0	1574	19	0
10	X	1581	0	1574	32	0
11	K	1576	0	1581	19	0
11	Y	1584	0	1590	36	0
12	L	1644	0	1595	35	0
12	Z	1644	0	1595	20	0
13	1	1757	0	1711	46	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	M	1757	0	1711	50	0
14	2	1824	0	1832	31	0
14	N	1824	0	1832	31	0
All	All	49360	0	49104	890	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 9.

The worst 5 of 890 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)
13:M:155:THR:HG21	13:M:159:VAL:HG12	1.35	1.05
13:M:18:THR:CG2	13:M:30:TYR:HA	1.90	1.01
8:H:1:THR:HG22	8:H:33:LYS:HZ3	1.26	0.99
7:U:11:MET:O	7:U:13:VAL:N	1.96	0.98
11:K:184:ASP:OD2	11:K:189:ARG:NH1	1.99	0.94

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	241/252 (96%)	234 (97%)	7 (3%)	0	100 100
1	O	241/252 (96%)	229 (95%)	12 (5%)	0	100 100
2	B	247/250 (99%)	240 (97%)	5 (2%)	2 (1%)	19 55
2	P	247/250 (99%)	229 (93%)	16 (6%)	2 (1%)	19 55
3	C	238/258 (92%)	227 (95%)	8 (3%)	3 (1%)	12 44
3	Q	242/258 (94%)	219 (90%)	18 (7%)	5 (2%)	7 33
4	D	239/254 (94%)	227 (95%)	5 (2%)	7 (3%)	4 25

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	R	239/254 (94%)	217 (91%)	16 (7%)	6 (2%)	5	29
5	E	235/260 (90%)	217 (92%)	15 (6%)	3 (1%)	12	44
5	S	234/260 (90%)	215 (92%)	12 (5%)	7 (3%)	4	24
6	F	230/234 (98%)	201 (87%)	23 (10%)	6 (3%)	5	28
6	T	230/234 (98%)	204 (89%)	18 (8%)	8 (4%)	3	21
7	G	235/277 (85%)	216 (92%)	18 (8%)	1 (0%)	34	68
7	U	235/277 (85%)	214 (91%)	17 (7%)	4 (2%)	9	38
8	H	194/215 (90%)	177 (91%)	15 (8%)	2 (1%)	15	51
8	V	197/215 (92%)	179 (91%)	15 (8%)	3 (2%)	10	41
9	I	220/261 (84%)	209 (95%)	9 (4%)	2 (1%)	17	53
9	W	220/261 (84%)	206 (94%)	13 (6%)	1 (0%)	29	65
10	J	202/205 (98%)	187 (93%)	13 (6%)	2 (1%)	15	51
10	X	202/205 (98%)	185 (92%)	17 (8%)	0	100	100
11	K	195/238 (82%)	183 (94%)	10 (5%)	2 (1%)	15	51
11	Y	196/238 (82%)	174 (89%)	18 (9%)	4 (2%)	7	34
12	L	210/287 (73%)	197 (94%)	12 (6%)	1 (0%)	29	65
12	Z	210/287 (73%)	198 (94%)	12 (6%)	0	100	100
13	1	220/241 (91%)	206 (94%)	14 (6%)	0	100	100
13	M	220/241 (91%)	204 (93%)	12 (6%)	4 (2%)	8	37
14	2	231/266 (87%)	210 (91%)	19 (8%)	2 (1%)	17	53
14	N	231/266 (87%)	212 (92%)	17 (7%)	2 (1%)	17	53
All	All	6281/6996 (90%)	5816 (93%)	386 (6%)	79 (1%)	12	44

5 of 79 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	184	MET
5	E	132	ARG
6	F	176	LEU
6	F	203	ASP
11	K	49	ALA

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	207/210 (99%)	193 (93%)	14 (7%)	16 46
1	O	207/210 (99%)	194 (94%)	13 (6%)	18 49
2	B	208/209 (100%)	197 (95%)	11 (5%)	22 55
2	P	208/209 (100%)	198 (95%)	10 (5%)	25 59
3	C	203/216 (94%)	187 (92%)	16 (8%)	12 40
3	Q	203/216 (94%)	184 (91%)	19 (9%)	8 30
4	D	213/226 (94%)	198 (93%)	15 (7%)	15 45
4	R	213/226 (94%)	196 (92%)	17 (8%)	12 39
5	E	196/215 (91%)	185 (94%)	11 (6%)	21 53
5	S	197/215 (92%)	184 (93%)	13 (7%)	16 47
6	F	191/193 (99%)	175 (92%)	16 (8%)	11 37
6	T	191/193 (99%)	177 (93%)	14 (7%)	14 43
7	G	196/230 (85%)	176 (90%)	20 (10%)	7 27
7	U	196/230 (85%)	179 (91%)	17 (9%)	10 34
8	H	162/178 (91%)	157 (97%)	5 (3%)	40 70
8	V	163/178 (92%)	158 (97%)	5 (3%)	40 70
9	I	181/214 (85%)	174 (96%)	7 (4%)	32 64
9	W	181/214 (85%)	177 (98%)	4 (2%)	52 77
10	J	172/173 (99%)	165 (96%)	7 (4%)	30 63
10	X	172/173 (99%)	164 (95%)	8 (5%)	26 60
11	K	174/209 (83%)	163 (94%)	11 (6%)	18 49
11	Y	175/209 (84%)	160 (91%)	15 (9%)	10 35
12	L	169/235 (72%)	159 (94%)	10 (6%)	19 51
12	Z	169/235 (72%)	161 (95%)	8 (5%)	26 60
13	1	185/201 (92%)	172 (93%)	13 (7%)	15 45
13	M	185/201 (92%)	172 (93%)	13 (7%)	15 45

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
14	2	199/224 (89%)	186 (94%)	13 (6%)	17 48
14	N	199/224 (89%)	191 (96%)	8 (4%)	31 64
All	All	5315/5866 (91%)	4982 (94%)	333 (6%)	18 49

5 of 333 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	S	177	GLU
11	Y	34	THR
6	T	72	LEU
7	U	153	SER
12	Z	9	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 132 such sidechains are listed below:

Mol	Chain	Res	Type
11	Y	190	GLN
12	Z	209	ASN
14	2	163	GLN
12	L	9	GLN
11	K	85	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)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	243/252 (96%)	-0.66	2 (0%) 86 78	29, 46, 74, 113	0
1	O	243/252 (96%)	-0.66	1 (0%) 92 89	32, 48, 72, 104	0
2	B	249/250 (99%)	-0.63	0 100 100	31, 49, 79, 105	0
2	P	249/250 (99%)	-0.55	0 100 100	36, 54, 81, 114	0
3	C	242/258 (93%)	-0.60	0 100 100	30, 50, 83, 106	0
3	Q	244/258 (94%)	-0.42	2 (0%) 86 78	31, 53, 96, 132	0
4	D	241/254 (94%)	-0.37	1 (0%) 92 89	33, 59, 106, 126	0
4	R	241/254 (94%)	-0.29	2 (0%) 86 78	38, 62, 108, 128	0
5	E	239/260 (91%)	-0.48	2 (0%) 86 78	31, 55, 80, 106	0
5	S	238/260 (91%)	-0.53	0 100 100	33, 57, 85, 121	0
6	F	232/234 (99%)	-0.41	1 (0%) 92 89	39, 60, 91, 121	0
6	T	232/234 (99%)	-0.43	1 (0%) 92 89	39, 60, 91, 123	0
7	G	237/277 (85%)	-0.57	1 (0%) 92 89	32, 55, 89, 119	0
7	U	237/277 (85%)	-0.51	0 100 100	34, 53, 89, 106	0
8	H	196/215 (91%)	-0.76	0 100 100	26, 40, 59, 80	0
8	V	199/215 (92%)	-0.70	2 (1%) 82 73	27, 40, 64, 130	0
9	I	222/261 (85%)	-0.70	0 100 100	31, 41, 62, 102	0
9	W	222/261 (85%)	-0.73	0 100 100	34, 47, 67, 106	0
10	J	204/205 (99%)	-0.74	1 (0%) 91 86	27, 43, 59, 84	0
10	X	204/205 (99%)	-0.71	0 100 100	29, 42, 66, 93	0
11	K	197/238 (82%)	-0.69	3 (1%) 73 61	26, 43, 65, 139	0
11	Y	198/238 (83%)	-0.70	1 (0%) 91 86	28, 44, 65, 125	0
12	L	212/287 (73%)	-0.71	0 100 100	26, 42, 58, 70	0
12	Z	212/287 (73%)	-0.75	0 100 100	27, 43, 62, 76	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
13	1	222/241 (92%)	-0.68	0	100	100	29, 44, 62, 90	0
13	M	222/241 (92%)	-0.72	0	100	100	28, 45, 67, 95	0
14	2	233/266 (87%)	-0.68	1 (0%)	92	89	27, 40, 55, 68	0
14	N	233/266 (87%)	-0.71	1 (0%)	92	89	30, 44, 63, 73	0
All	All	6343/6996 (90%)	-0.60	22 (0%)	94	92	26, 48, 82, 139	0

The worst 5 of 22 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
11	Y	197	GLN	3.9
8	V	-2	SER	3.8
5	E	127	ALA	3.3
6	T	6	TYR	3.2
4	R	207	ALA	3.2

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)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.