wwPDB X-ray Structure Validation Summary Report (i)

Mar 10, 2025 – 12:55 PM EDT

PDB ID	:	9AW3
Title	:	Yeast 20S proteasome soaked with MA9 crude extract
Authors	:	Meneghello, R.; Rustiguel, J.K.; Fernandes, A.Z.N.; Trivella, D.B.B.
Deposited on	:	2024-03-05
Resolution	:	3.42 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 (1)) were used in the production of this report:

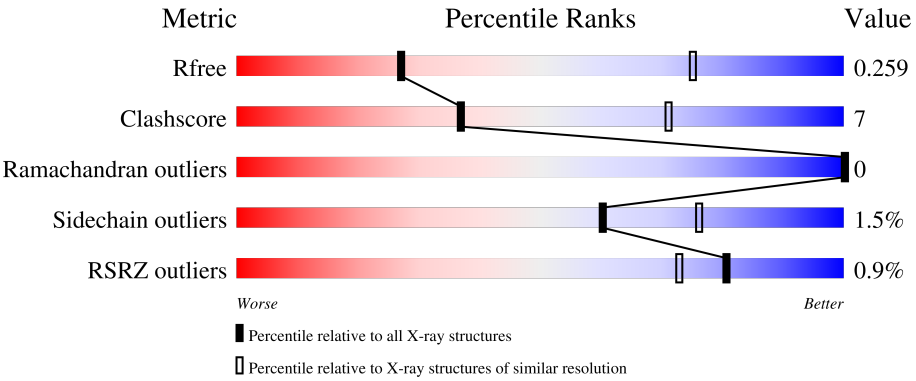
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41.4

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 3.42 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}	164625	1112 (3.48-3.36)
Clashscore	180529	1144 (3.48-3.36)
Ramachandran outliers	177936	1146 (3.48-3.36)
Sidechain outliers	177891	1146 (3.48-3.36)
RSRZ outliers	164620	1112 (3.48-3.36)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	250	78% 21%
1	O	250	82% 17%
2	B	258	2% 74% 19% 6%
2	P	258	2% 73% 20% 5%
3	C	254	% 76% 19%

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Mol	Chain	Length	Quality of chain
3	Q	254	2% 71% 23% • 5%
4	D	260	% 78% 13% 9%
4	R	260	81% 10% 9%
5	E	234	% 76% 21% ••
5	S	234	2% 77% 20% ••
6	F	287	2% 71% 14% 15%
6	T	287	% 70% 15% 15%
7	G	252	2% 83% 13% •
7	U	252	79% 17% •
8	H	232	83% 13% •
8	V	232	82% 12% • 5%
9	I	205	% 78% 22%
9	W	205	80% 20%
10	J	198	% 70% 29% •
10	X	198	76% 21% ••
11	K	212	86% 13%
11	Y	212	90% 9%
12	L	222	83% 17%
12	Z	222	83% 17%
13	M	233	76% 24% •
13	a	233	% 99% •
14	N	196	% 80% 19% •
14	b	196	% 99% •

2 Entry composition (i)

There are 17 unique types of molecules in this entry. The entry contains 49260 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
1	A	248	Total	C	N	O	S	0	0	0
			1897	1207	313	374	3			
1	O	249	Total	C	N	O	S	0	0	0
			1907	1214	314	376	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	243	Total	C	N	O	S	0	0	0
			1893	1198	315	377	3			
2	P	244	Total	C	N	O	S	0	0	0
			1909	1206	322	378	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	243	Total	C	N	O	S	0	0	0
			1910	1193	333	380	4			
3	Q	241	Total	C	N	O	S	0	0	0
			1853	1157	325	367	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	237	Total	C	N	O	S	0	0	0
			1833	1147	309	370	7			
4	R	236	Total	C	N	O	S	0	0	0
			1718	1075	290	346	7			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	231	Total	C	N	O	S	0	0	0
			1745	1095	301	345	4			
5	S	232	Total	C	N	O	S	0	0	0
			1774	1114	307	349	4			

- Molecule 6 is a protein called PRE10 isoform 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	244	Total	C	N	O	S	0	0	0
			1896	1205	330	357	4			
6	T	245	Total	C	N	O	S	0	0	0
			1884	1198	328	354	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	242	Total	C	N	O	S	0	0	0
			1904	1211	320	365	8			
7	U	242	Total	C	N	O	S	0	0	0
			1910	1215	318	369	8			

- Molecule 8 is a protein called proteasome endopeptidase complex.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	222	Total	C	N	O	S	0	0	0
			1684	1061	293	323	7			
8	V	221	Total	C	N	O	S	0	0	0
			1656	1045	284	320	7			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	204	Total	C	N	O	S	0	0	0
			1569	1003	257	301	8			
9	W	204	Total	C	N	O	S	0	0	0
			1581	1010	258	305	8			

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

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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	X	195	Total	C	N	O	S	0	0	0
			1547	984	262	295	6			

- Molecule 11 is a protein called proteasome endopeptidase complex.

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

- Molecule 12 is a protein called PRE7 isoform 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	222	Total	C	N	O	S	0	0	0
			1757	1115	303	335	4			
12	Z	222	Total	C	N	O	S	0	0	0
			1749	1110	302	333	4			

- Molecule 13 is a protein called Proteasome subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	233	Total	C	N	O	S	0	0	0
			1824	1154	312	351	7			
13	a	233	Total	C	N	O	S	0	0	0
			1809	1142	310	350	7			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	N	196	Total	C	N	O	S	0	0	0
			1508	952	249	300	7			
14	b	196	Total	C	N	O	S	0	0	0
			1495	945	245	298	7			

- Molecule 15 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	H	1	Total	Mg	0	0
			1	1		
15	I	1	Total	Mg	0	0
			1	1		

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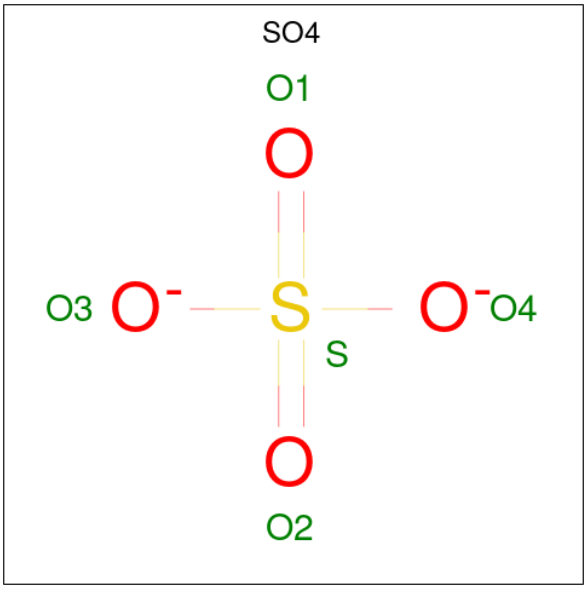
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	L	1	Total Mg 1 1	0	0
15	V	1	Total Mg 1 1	0	0
15	W	1	Total Mg 1 1	0	0
15	Y	1	Total Mg 1 1	0	0
15	Z	1	Total Mg 1 1	0	0

- Molecule 16 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	M	1	Total O S 5 4 1	0	0
16	a	1	Total O S 5 4 1	0	0
16	a	1	Total O S 5 4 1	0	0

- Molecule 17 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	A	5	Total O 5 5	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	B	12	Total O 12 12	0	0
17	C	5	Total O 5 5	0	0
17	D	5	Total O 5 5	0	0
17	E	4	Total O 4 4	0	0
17	F	8	Total O 8 8	0	0
17	G	2	Total O 2 2	0	0
17	O	5	Total O 5 5	0	0
17	P	8	Total O 8 8	0	0
17	Q	11	Total O 11 11	0	0
17	R	1	Total O 1 1	0	0
17	S	4	Total O 4 4	0	0
17	T	3	Total O 3 3	0	0
17	U	5	Total O 5 5	0	0
17	H	12	Total O 12 12	0	0
17	I	3	Total O 3 3	0	0
17	J	6	Total O 6 6	0	0
17	K	2	Total O 2 2	0	0
17	L	5	Total O 5 5	0	0
17	M	12	Total O 12 12	0	0
17	N	6	Total O 6 6	0	0
17	V	12	Total O 12 12	0	0

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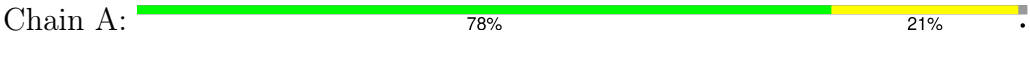
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	W	2	Total O 2 2	0	0
17	X	10	Total O 10 10	0	0
17	Y	7	Total O 7 7	0	0
17	Z	6	Total O 6 6	0	0
17	a	14	Total O 14 14	0	0
17	b	2	Total O 2 2	0	0

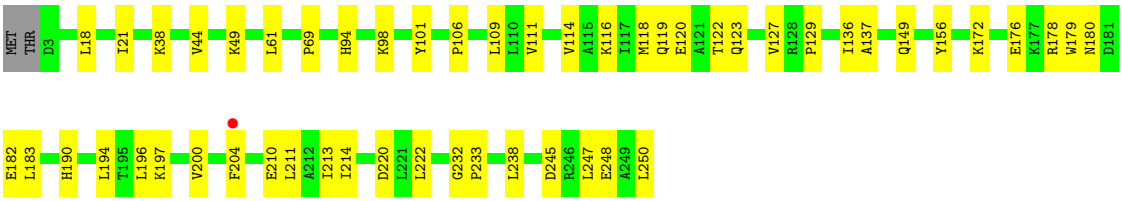
3 Residue-property plots (i)

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

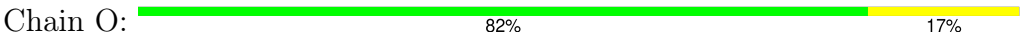
Chain A:

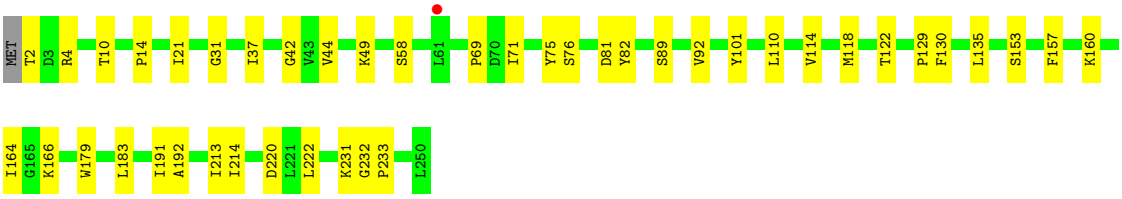




• Molecule 1: Proteasome subunit alpha type-2

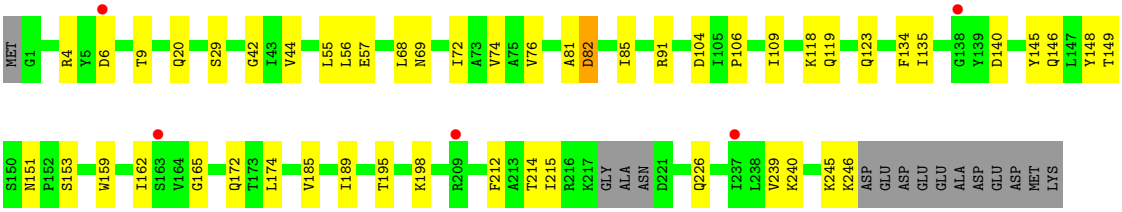
Chain O:





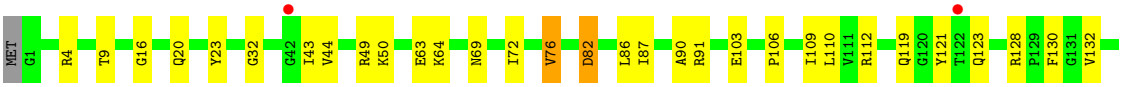
• Molecule 2: Proteasome subunit alpha type-3

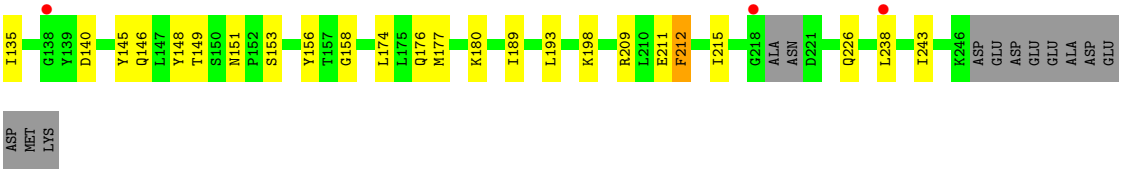
Chain B:



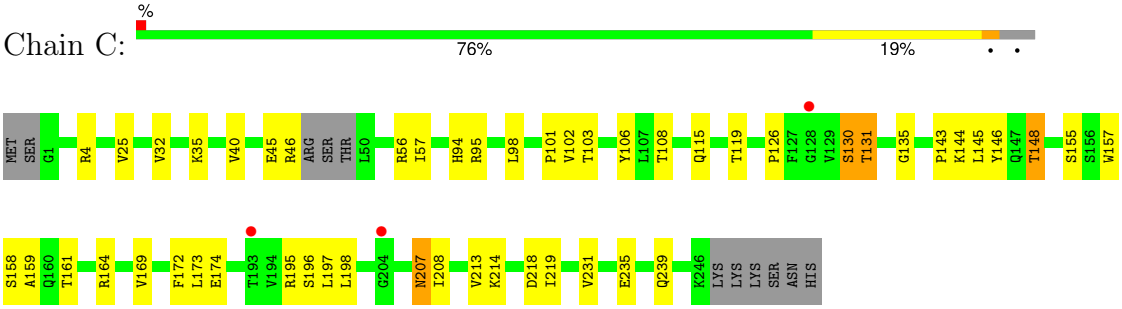
• Molecule 2: Proteasome subunit alpha type-3

Chain P:

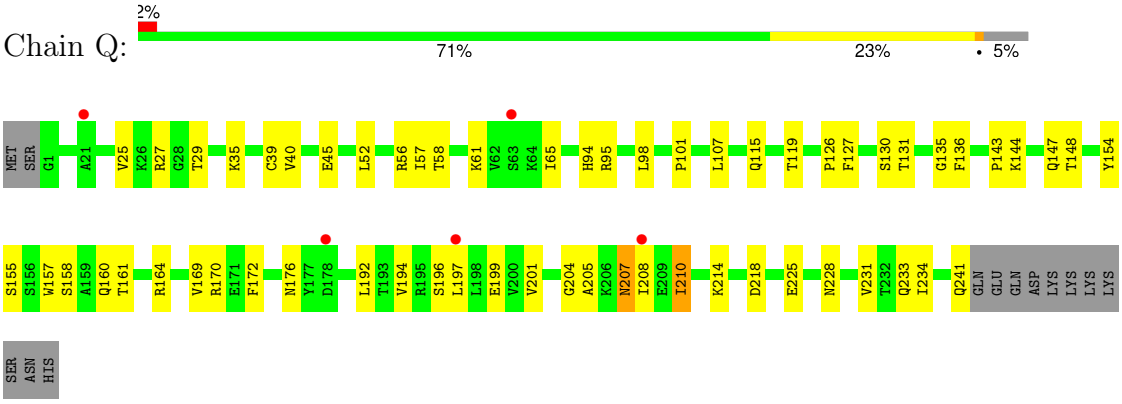




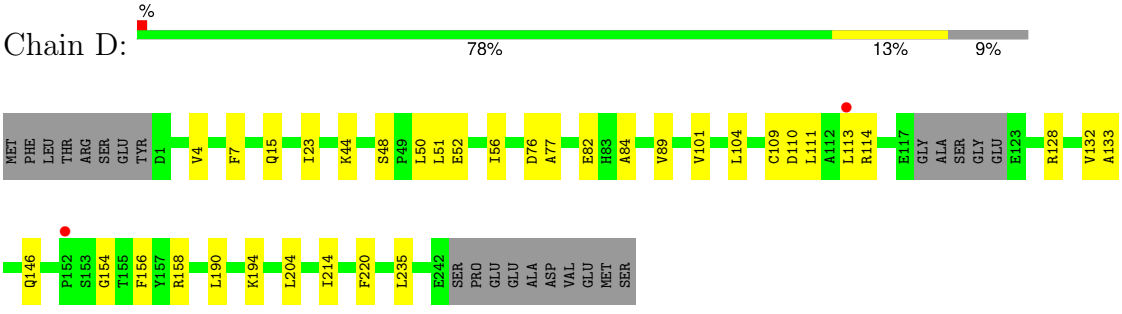
• Molecule 3: Proteasome subunit alpha type-4



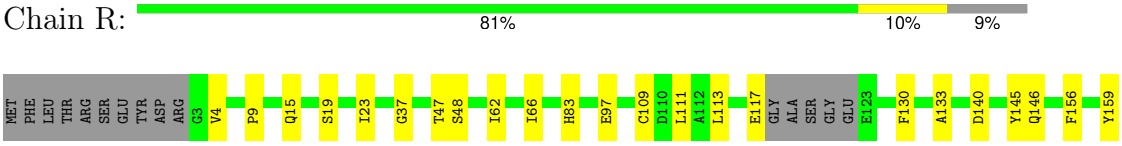
• Molecule 3: Proteasome subunit alpha type-4

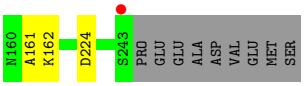


• Molecule 4: Proteasome subunit alpha type-5

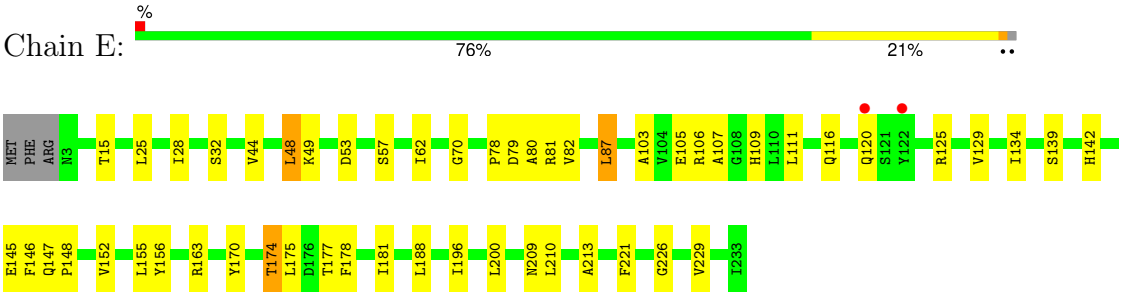


• Molecule 4: Proteasome subunit alpha type-5

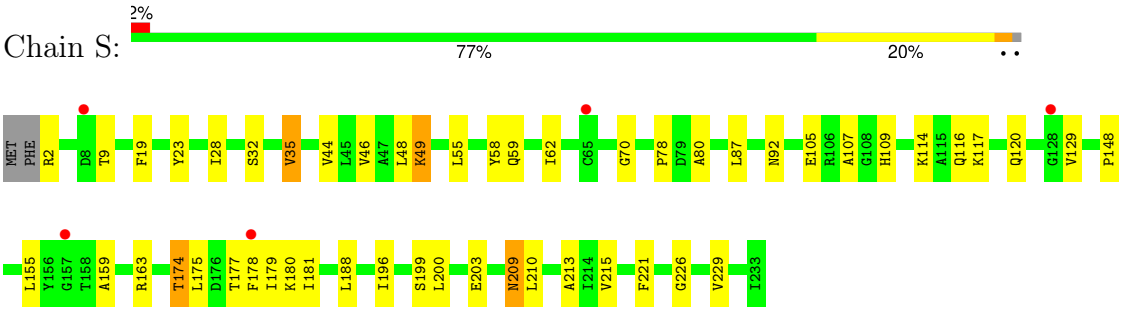




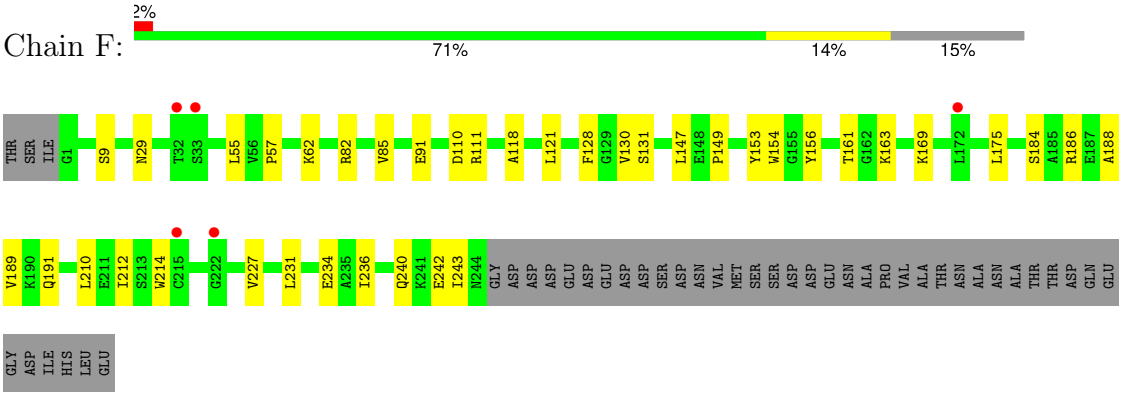
• Molecule 5: Proteasome subunit alpha type-6



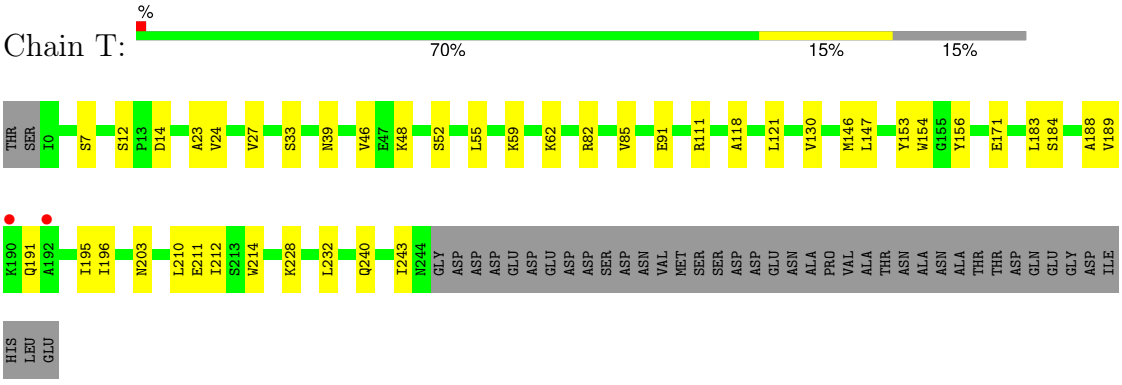
• Molecule 5: Proteasome subunit alpha type-6



• Molecule 6: PRE10 isoform 1

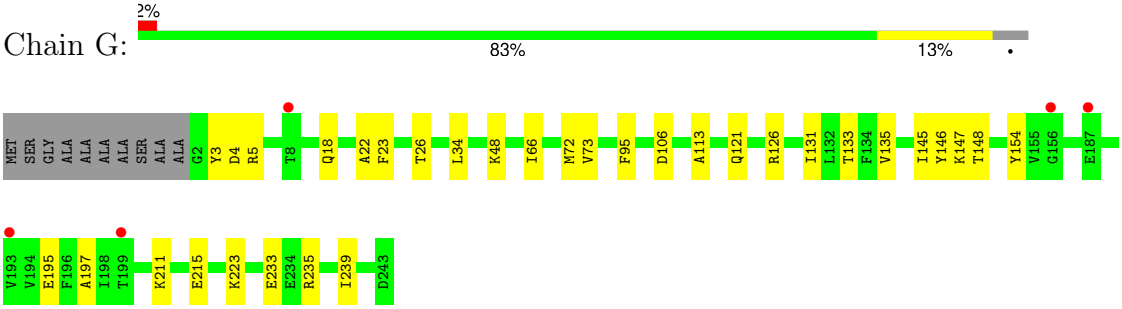


• Molecule 6: PRE10 isoform 1



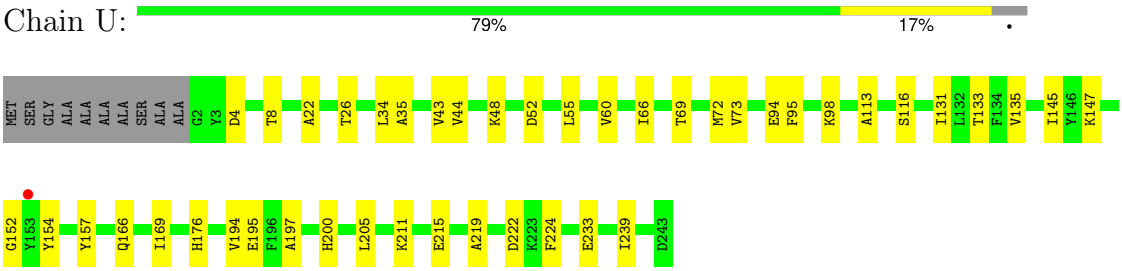
• Molecule 7: Proteasome subunit alpha type-1

Chain G:



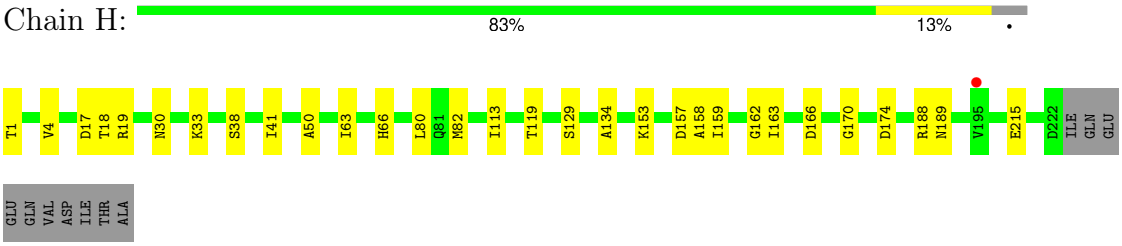
• Molecule 7: Proteasome subunit alpha type-1

Chain U:



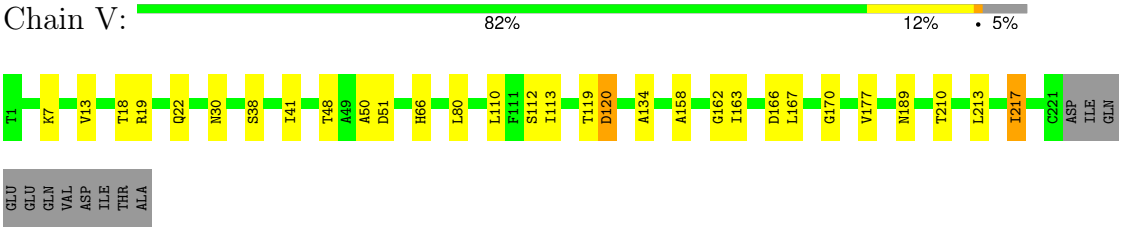
• Molecule 8: proteasome endopeptidase complex

Chain H:



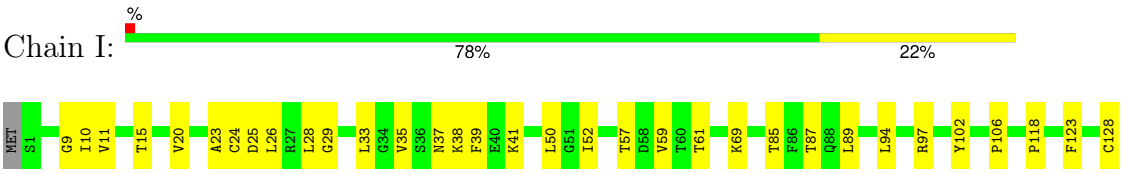
• Molecule 8: proteasome endopeptidase complex

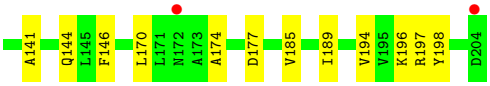
Chain V:



• Molecule 9: Proteasome subunit beta type-3

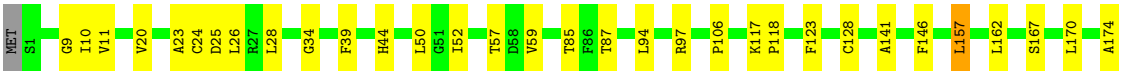
Chain I:

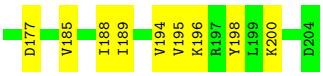




• Molecule 9: Proteasome subunit beta type-3

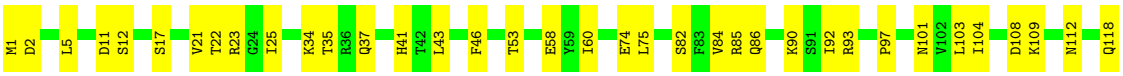
Chain W:

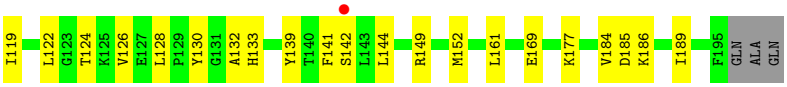




• Molecule 10: Proteasome subunit beta type-4

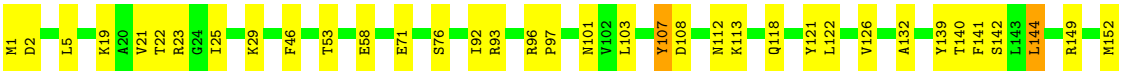
Chain J:





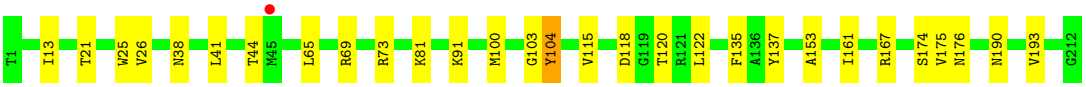
• Molecule 10: Proteasome subunit beta type-4

Chain X:



• Molecule 11: proteasome endopeptidase complex

Chain K:

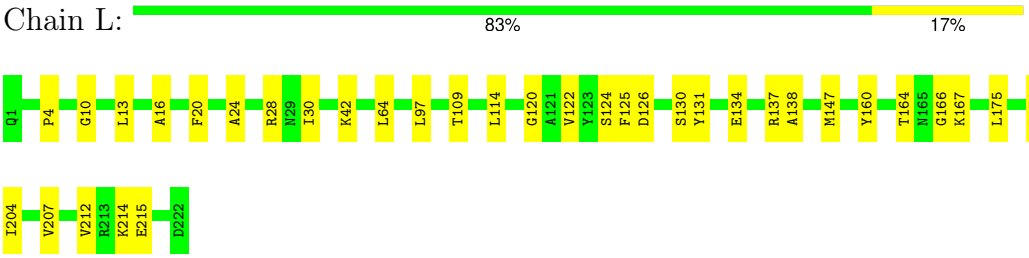


• Molecule 11: proteasome endopeptidase complex

Chain Y:

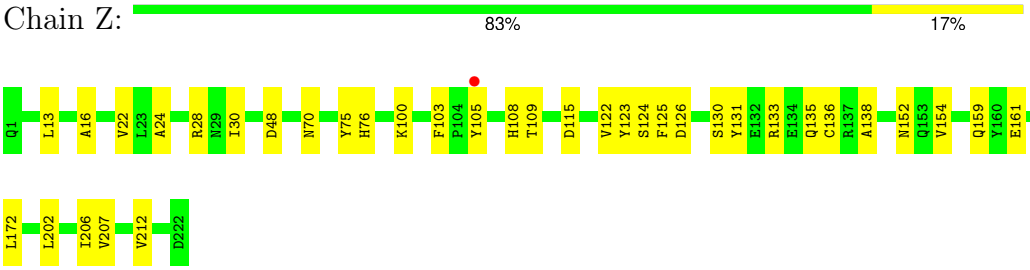
• Molecule 12: PRE7 isoform 1

Chain L:



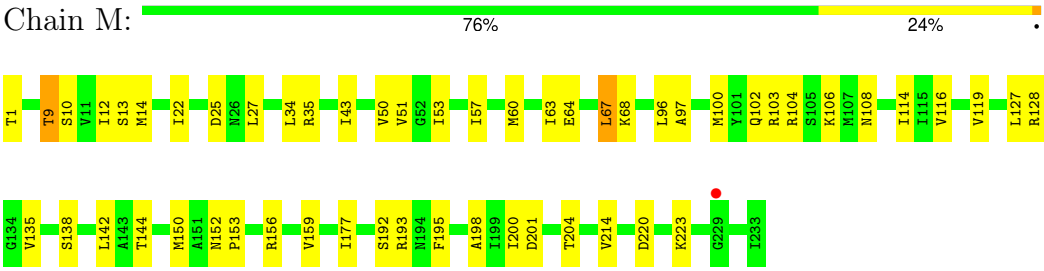
• Molecule 12: PRE7 isoform 1

Chain Z:



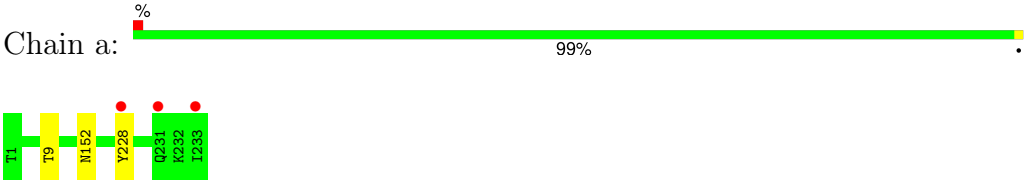
• Molecule 13: Proteasome subunit beta

Chain M:



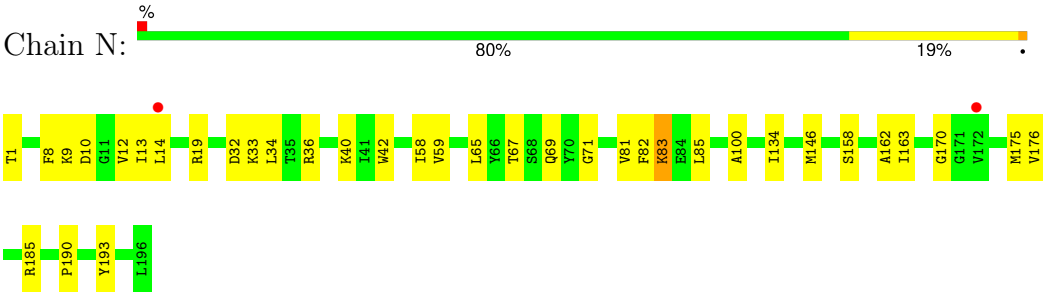
• Molecule 13: Proteasome subunit beta

Chain a:



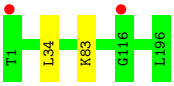
• Molecule 14: Proteasome subunit beta type-1

Chain N:



• Molecule 14: Proteasome subunit beta type-1

Chain b:


T1
L34
K83
G116
L196

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	131.96Å 301.46Å 142.65Å 90.00° 111.98° 90.00°	Depositor
Resolution (Å)	29.84 – 3.42 29.84 – 3.42	Depositor EDS
% Data completeness (in resolution range)	98.4 (29.84-3.42) 84.3 (29.84-3.42)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.59 (at 3.39Å)	Xtriage
Refinement program	PHENIX 1.21-5207	Depositor
R, R_{free}	0.215 , 0.259 0.215 , 0.259	Depositor DCC
R_{free} test set	7065 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	69.4	Xtriage
Anisotropy	1.024	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 78.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	49260	wwPDB-VP
Average B, all atoms (Å^2)	100.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.55% 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: SO4, MG

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	0.25	0/1934	0.47	0/2618
1	O	0.25	0/1944	0.46	0/2632
2	B	0.24	0/1922	0.47	0/2600
2	P	0.24	0/1938	0.49	0/2619
3	C	0.24	0/1938	0.49	0/2621
3	Q	0.25	0/1881	0.50	0/2551
4	D	0.24	0/1857	0.47	0/2501
4	R	0.24	0/1742	0.45	0/2365
5	E	0.24	0/1771	0.48	0/2399
5	S	0.24	0/1801	0.48	0/2436
6	F	0.25	0/1936	0.47	0/2614
6	T	0.25	0/1924	0.47	0/2603
7	G	0.24	0/1942	0.46	0/2631
7	U	0.25	0/1948	0.46	0/2638
8	H	0.23	0/1715	0.46	0/2326
8	V	0.24	0/1687	0.45	0/2293
9	I	0.25	0/1599	0.48	0/2160
9	W	0.25	0/1611	0.48	0/2174
10	J	0.24	0/1589	0.47	0/2142
10	X	0.24	0/1575	0.48	0/2126
11	K	0.24	0/1681	0.47	0/2274
11	Y	0.24	0/1681	0.47	0/2274
12	L	0.25	0/1795	0.48	0/2420
12	Z	0.25	0/1787	0.48	0/2411
13	M	0.25	0/1855	0.49	0/2514
13	a	0.25	0/1840	0.49	0/2498
14	N	0.24	0/1537	0.47	0/2083
14	b	0.25	0/1524	0.48	0/2068
All	All	0.24	0/49954	0.47	0/67591

There are no bond length outliers.

There are no bond angle outliers.

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	1897	0	1901	31	0
1	O	1907	0	1917	24	0
2	B	1893	0	1893	33	0
2	P	1909	0	1918	35	0
3	C	1910	0	1916	34	0
3	Q	1853	0	1837	39	0
4	D	1833	0	1816	24	0
4	R	1718	0	1594	17	0
5	E	1745	0	1722	32	0
5	S	1774	0	1766	34	0
6	F	1896	0	1889	23	0
6	T	1884	0	1859	27	0
7	G	1904	0	1886	23	0
7	U	1910	0	1894	23	0
8	H	1684	0	1688	18	0
8	V	1656	0	1640	19	0
9	I	1569	0	1555	30	0
9	W	1581	0	1574	28	0
10	J	1561	0	1569	38	0
10	X	1547	0	1543	31	0
11	K	1644	0	1595	20	0
11	Y	1644	0	1595	13	0
12	L	1757	0	1711	21	0
12	Z	1749	0	1696	22	0
13	M	1824	0	1832	37	0
13	a	1809	0	1792	0	0
14	N	1508	0	1470	22	0
14	b	1495	0	1446	0	0
15	H	1	0	0	0	0
15	I	1	0	0	0	0
15	L	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	V	1	0	0	0	0
15	W	1	0	0	0	0
15	Y	1	0	0	0	0
15	Z	1	0	0	0	0
16	M	5	0	0	0	0
16	a	10	0	0	0	0
17	A	5	0	0	0	0
17	B	12	0	0	0	0
17	C	5	0	0	0	0
17	D	5	0	0	0	0
17	E	4	0	0	0	0
17	F	8	0	0	0	0
17	G	2	0	0	0	0
17	H	12	0	0	0	0
17	I	3	0	0	0	0
17	J	6	0	0	0	0
17	K	2	0	0	0	0
17	L	5	0	0	0	0
17	M	12	0	0	1	0
17	N	6	0	0	0	0
17	O	5	0	0	0	0
17	P	8	0	0	0	0
17	Q	11	0	0	0	0
17	R	1	0	0	0	0
17	S	4	0	0	0	0
17	T	3	0	0	0	0
17	U	5	0	0	0	0
17	V	12	0	0	1	0
17	W	2	0	0	0	0
17	X	10	0	0	0	0
17	Y	7	0	0	1	0
17	Z	6	0	0	0	0
17	a	14	0	0	0	0
17	b	2	0	0	0	0
All	All	49260	0	48514	628	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 7.

The worst 5 of 628 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)
3:C:135:GLY:O	3:C:144:LYS:HB2	1.73	0.87
1:A:38:LYS:NZ	2:B:57:GLU:OE1	2.16	0.77
2:P:63:GLU:HG3	2:P:64:LYS:HG2	1.69	0.74
10:X:92:ILE:HA	10:X:97:PRO:HB3	1.70	0.73
5:S:80:ALA:HB2	5:S:129:VAL:HG21	1.72	0.72

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	246/250 (98%)	241 (98%)	5 (2%)	0	100	100
1	O	247/250 (99%)	242 (98%)	5 (2%)	0	100	100
2	B	239/258 (93%)	233 (98%)	6 (2%)	0	100	100
2	P	240/258 (93%)	234 (98%)	6 (2%)	0	100	100
3	C	239/254 (94%)	233 (98%)	6 (2%)	0	100	100
3	Q	239/254 (94%)	233 (98%)	6 (2%)	0	100	100
4	D	233/260 (90%)	227 (97%)	6 (3%)	0	100	100
4	R	232/260 (89%)	228 (98%)	4 (2%)	0	100	100
5	E	229/234 (98%)	225 (98%)	4 (2%)	0	100	100
5	S	230/234 (98%)	225 (98%)	5 (2%)	0	100	100
6	F	242/287 (84%)	234 (97%)	8 (3%)	0	100	100
6	T	243/287 (85%)	236 (97%)	7 (3%)	0	100	100
7	G	240/252 (95%)	230 (96%)	10 (4%)	0	100	100
7	U	240/252 (95%)	229 (95%)	11 (5%)	0	100	100
8	H	220/232 (95%)	212 (96%)	8 (4%)	0	100	100
8	V	219/232 (94%)	213 (97%)	6 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	I	202/205 (98%)	190 (94%)	12 (6%)	0	100	100
9	W	202/205 (98%)	191 (95%)	11 (5%)	0	100	100
10	J	193/198 (98%)	189 (98%)	4 (2%)	0	100	100
10	X	193/198 (98%)	189 (98%)	4 (2%)	0	100	100
11	K	210/212 (99%)	201 (96%)	9 (4%)	0	100	100
11	Y	210/212 (99%)	203 (97%)	7 (3%)	0	100	100
12	L	220/222 (99%)	213 (97%)	7 (3%)	0	100	100
12	Z	220/222 (99%)	214 (97%)	6 (3%)	0	100	100
13	M	231/233 (99%)	220 (95%)	11 (5%)	0	100	100
13	a	231/233 (99%)	219 (95%)	12 (5%)	0	100	100
14	N	194/196 (99%)	189 (97%)	5 (3%)	0	100	100
14	b	194/196 (99%)	190 (98%)	4 (2%)	0	100	100
All	All	6278/6586 (95%)	6083 (97%)	195 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	206/209 (99%)	205 (100%)	1 (0%)	86	92
1	O	208/209 (100%)	206 (99%)	2 (1%)	73	83
2	B	202/216 (94%)	197 (98%)	5 (2%)	42	65
2	P	204/216 (94%)	198 (97%)	6 (3%)	37	61
3	C	215/226 (95%)	211 (98%)	4 (2%)	52	71
3	Q	204/226 (90%)	200 (98%)	4 (2%)	50	70
4	D	196/215 (91%)	195 (100%)	1 (0%)	86	92
4	R	167/215 (78%)	165 (99%)	2 (1%)	67	79
5	E	184/193 (95%)	179 (97%)	5 (3%)	40	63

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	S	189/193 (98%)	184 (97%)	5 (3%)	41	64
6	F	201/238 (84%)	197 (98%)	4 (2%)	50	70
6	T	197/238 (83%)	194 (98%)	3 (2%)	60	76
7	G	204/210 (97%)	204 (100%)	0	100	100
7	U	206/210 (98%)	204 (99%)	2 (1%)	73	83
8	H	181/190 (95%)	180 (99%)	1 (1%)	84	90
8	V	176/190 (93%)	173 (98%)	3 (2%)	56	74
9	I	169/173 (98%)	166 (98%)	3 (2%)	54	73
9	W	172/173 (99%)	168 (98%)	4 (2%)	45	67
10	J	173/175 (99%)	171 (99%)	2 (1%)	67	79
10	X	169/175 (97%)	163 (96%)	6 (4%)	30	55
11	K	169/169 (100%)	167 (99%)	2 (1%)	67	79
11	Y	169/169 (100%)	167 (99%)	2 (1%)	67	79
12	L	185/185 (100%)	185 (100%)	0	100	100
12	Z	183/185 (99%)	182 (100%)	1 (0%)	86	92
13	M	199/199 (100%)	196 (98%)	3 (2%)	60	76
13	a	195/199 (98%)	192 (98%)	3 (2%)	60	76
14	N	161/162 (99%)	158 (98%)	3 (2%)	52	71
14	b	158/162 (98%)	156 (99%)	2 (1%)	65	78
All	All	5242/5520 (95%)	5163 (98%)	79 (2%)	60	76

5 of 79 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
14	N	178	LEU
11	Y	104	TYR
8	V	189	ASN
10	X	21	VAL
13	a	152	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
4	R	146	GLN
14	N	161	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 10 ligands modelled in this entry, 7 are monoatomic - leaving 3 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	$\#\|Z\| > 2$
16	SO4	a	301	-	4,4,4	0.67	0	6,6,6	0.07	0
16	SO4	M	301	-	4,4,4	0.67	0	6,6,6	0.09	0
16	SO4	a	302	-	4,4,4	0.67	0	6,6,6	0.08	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.

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

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	248/250 (99%)	0.18	1 (0%) 89 87	65, 98, 134, 168	0
1	O	249/250 (99%)	0.14	1 (0%) 89 87	63, 100, 137, 166	0
2	B	243/258 (94%)	0.28	5 (2%) 63 54	70, 108, 146, 165	0
2	P	244/258 (94%)	0.37	5 (2%) 64 56	64, 100, 135, 158	0
3	C	243/254 (95%)	0.28	3 (1%) 76 68	66, 104, 155, 179	0
3	Q	241/254 (94%)	0.40	5 (2%) 63 54	65, 112, 152, 184	0
4	D	237/260 (91%)	0.21	2 (0%) 82 75	66, 101, 131, 155	0
4	R	236/260 (90%)	0.34	1 (0%) 89 87	72, 114, 142, 170	0
5	E	231/234 (98%)	0.39	2 (0%) 81 73	72, 116, 155, 175	0
5	S	232/234 (99%)	0.43	5 (2%) 62 53	68, 114, 164, 182	0
6	F	244/287 (85%)	0.38	5 (2%) 64 56	60, 106, 144, 161	0
6	T	245/287 (85%)	0.26	2 (0%) 82 75	61, 98, 135, 156	0
7	G	242/252 (96%)	0.30	5 (2%) 63 54	58, 96, 126, 183	0
7	U	242/252 (96%)	0.23	1 (0%) 89 87	62, 94, 131, 164	0
8	H	222/232 (95%)	0.17	1 (0%) 87 83	52, 96, 125, 184	0
8	V	221/232 (95%)	0.17	0 100 100	64, 95, 119, 157	0
9	I	204/205 (99%)	0.23	2 (0%) 79 71	63, 94, 123, 139	0
9	W	204/205 (99%)	0.14	0 100 100	60, 85, 116, 140	0
10	J	195/198 (98%)	0.15	1 (0%) 87 83	63, 90, 117, 154	0
10	X	195/198 (98%)	0.16	0 100 100	57, 84, 110, 132	0
11	K	212/212 (100%)	0.14	1 (0%) 87 83	59, 87, 115, 132	0
11	Y	212/212 (100%)	0.28	0 100 100	67, 99, 127, 143	0
12	L	222/222 (100%)	0.15	0 100 100	64, 92, 121, 160	0
12	Z	222/222 (100%)	0.32	1 (0%) 87 83	69, 99, 135, 150	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å^2)	Q<0.9
13	M	233/233 (100%)	0.23	1 (0%)	89 87	64, 94, 136, 160	0
13	a	233/233 (100%)	0.23	3 (1%)	74 66	58, 86, 128, 164	0
14	N	196/196 (100%)	0.20	2 (1%)	79 71	62, 86, 117, 135	0
14	b	196/196 (100%)	0.22	2 (1%)	79 71	59, 86, 114, 135	0
All	All	6344/6586 (96%)	0.25	57 (0%)	81 73	52, 97, 140, 184	0

The worst 5 of 57 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
13	a	233	ILE	3.7
14	N	172	VAL	3.5
3	C	193	THR	3.0
2	P	218	GLY	3.0
7	G	187	GLU	2.8

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
15	MG	W	301	1/1	0.63	0.14	72,72,72,72	0
16	SO4	a	301	5/5	0.81	0.17	70,89,104,113	5
16	SO4	a	302	5/5	0.82	0.25	100,106,147,171	0
15	MG	Z	301	1/1	0.83	0.08	68,68,68,68	0
15	MG	Y	301	1/1	0.86	0.08	114,114,114,114	0
15	MG	I	301	1/1	0.88	0.13	87,87,87,87	0
15	MG	L	301	1/1	0.89	0.16	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
16	SO4	M	301	5/5	0.89	0.26	108,113,168,170	0
15	MG	V	301	1/1	0.90	0.12	100,100,100,100	0
15	MG	H	301	1/1	0.96	0.10	113,113,113,113	0

6.5 Other polymers (i)

There are no such residues in this entry.