



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 22, 2025 – 01:53 pm BST

PDB ID : 9FRW / pdb\_00009frw  
Title : Yeast 20S proteasome with human beta1i (1-51)  
Authors : Maurits, E.; Huber, E.M.; Decker, P.M.; Wang, X.; Heinemeyer, W.; Florea, B.I.; Groll, M.; Overkleedt, H.S.  
Deposited on : 2024-06-19  
Resolution : 2.85 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](mailto: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 ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.42

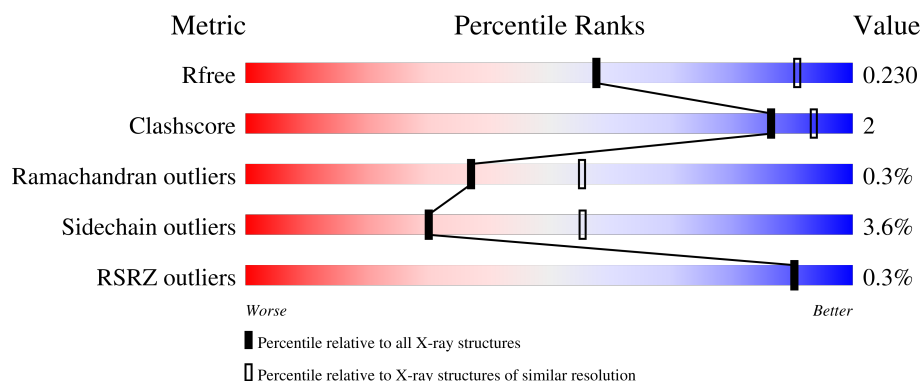
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

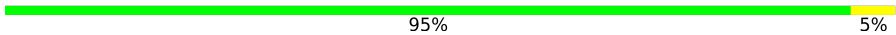

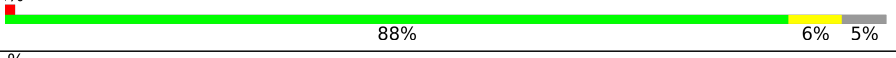
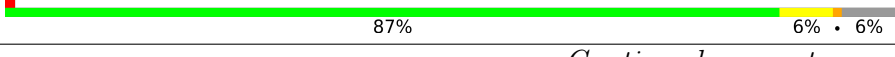
The reported resolution of this entry is 2.85 Å.

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.














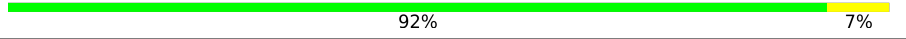
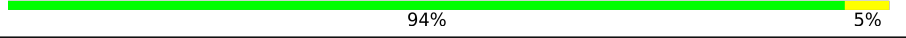
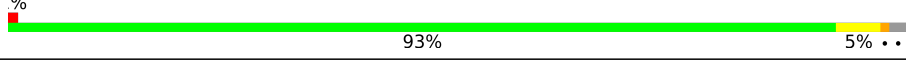


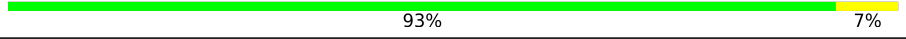
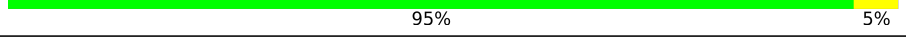
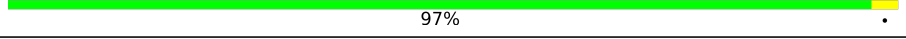



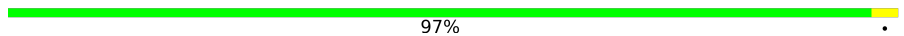
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	164625	1268 (2.88-2.84)
Clashscore	180529	1351 (2.88-2.84)
Ramachandran outliers	177936	1318 (2.88-2.84)
Sidechain outliers	177891	1319 (2.88-2.84)
RSRZ outliers	164620	1269 (2.88-2.84)

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  $\geq 3$ , 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  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	250	 97% .
1	O	250	 95% 5%
2	B	258	 % 88% 7% 5%
2	P	258	 % 88% 6% 5%
3	C	254	 % 87% 6% . 6%

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Mol	Chain	Length	Quality of chain
3	Q	254	 89% 6%
4	D	260	 85% 10%
4	R	260	 85% 5% 10%
5	E	234	 91% 7% ..
5	S	234	 90% 8% .
6	F	288	 78% 6% 16%
6	T	288	 78% 6% 16%
7	G	252	 90% 6% .
7	U	252	 89% 6% .
8	H	232	 89% 8% .
8	V	232	 88% 8% . .
9	I	205	 92% 7%
9	W	205	 94% 5%
10	J	198	 93% 5% ..
10	X	198	 91% 7% ..
11	K	212	 91% 8% .
11	Y	212	 93% 7%
12	L	222	 95% 5%
12	Z	222	 97% .
13	M	246	 84% 7% . 9%
13	a	246	 89% . 7%
14	N	196	 91% 8% .
14	b	196	 97% .

## 2 Entry composition

There are 19 unique types of molecules in this entry. The entry contains 49457 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	250	Total	C	N	O	S	0	0	0
			1915	1219	315	377	4			
1	O	250	Total	C	N	O	S	0	0	0
			1915	1219	315	377	4			

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	235	Total	C	N	O	S	0	0	0
			1813	1136	304	366	7			
4	R	235	Total	C	N	O	S	0	0	0
			1813	1136	304	366	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
			1773	1114	307	348	4			
5	S	231	Total	C	N	O	S	0	0	0
			1773	1114	307	348	4			

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	226	Total	C	N	O	S	0	0	0
			1719	1082	298	332	7			
8	V	226	Total	C	N	O	S	0	1	0
			1727	1086	300	334	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
			1581	1010	258	305	8			
9	W	204	Total	C	N	O	S	0	0	0
			1581	1010	258	305	8			

- Molecule 10 is a protein called Proteasome 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
			1561	992	264	299	6			

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	225	Total	C	N	O	S	0	0	0
			1761	1114	301	339	7			
13	a	228	Total	C	N	O	S	0	0	0
			1786	1131	305	343	7			

- Molecule 14 is a protein called Proteasome subunit beta type-9, Proteasome subunit beta type-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	N	196	Total	C	N	O	S	0	0	0
			1502	950	244	301	7			
14	b	196	Total	C	N	O	S	0	0	0
			1502	950	244	301	7			

- Molecule 15 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

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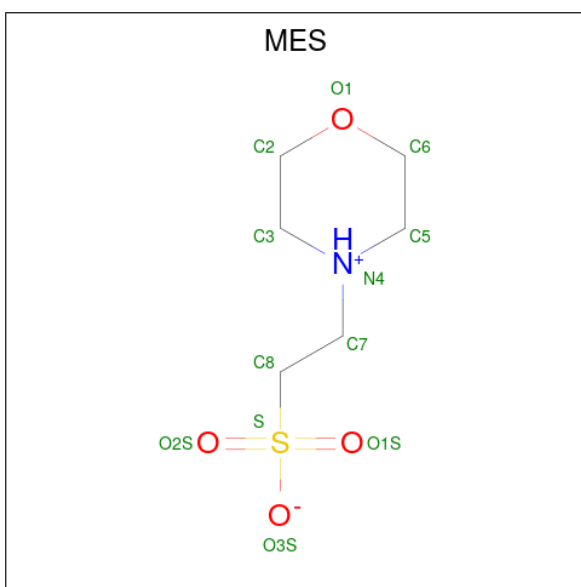
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	H	1	Total 1	Cl 1	0	0
15	I	1	Total 1	Cl 1	0	0
15	L	1	Total 1	Cl 1	0	0
15	U	2	Total 2	Cl 2	0	0
15	V	1	Total 1	Cl 1	0	0

- Molecule 16 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

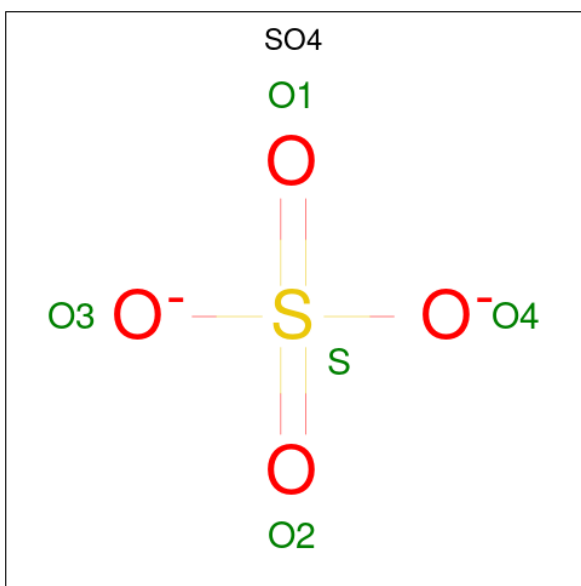
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	G	1	Total 1	Mg 1	0	0
16	I	1	Total 1	Mg 1	0	0
16	K	1	Total 1	Mg 1	0	0
16	N	1	Total 1	Mg 1	0	0
16	U	1	Total 1	Mg 1	0	0
16	V	1	Total 1	Mg 1	0	0
16	W	1	Total 1	Mg 1	0	0
16	Y	1	Total 1	Mg 1	0	0
16	Z	1	Total 1	Mg 1	0	0

- Molecule 17 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: C<sub>6</sub>H<sub>13</sub>NO<sub>4</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
17	M	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
17	a	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 18 is SULFATE ION (CCD ID: SO<sub>4</sub>) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
18	N	1	Total	O	S	0	0
			5	4	1		
18	b	1	Total	O	S	0	0
			5	4	1		



- Molecule 19 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
19	A	4	Total O 4 4	0	0
19	B	8	Total O 8 8	0	0
19	C	6	Total O 6 6	0	0
19	D	6	Total O 6 6	0	0
19	E	6	Total O 6 6	0	0
19	F	1	Total O 1 1	0	0
19	G	6	Total O 6 6	0	0
19	H	5	Total O 5 5	0	0
19	I	3	Total O 3 3	0	0
19	J	8	Total O 8 8	0	0
19	K	13	Total O 13 13	0	0
19	L	7	Total O 7 7	0	0
19	M	9	Total O 9 9	0	0
19	N	2	Total O 2 2	0	0
19	O	3	Total O 3 3	0	0
19	P	4	Total O 4 4	0	0
19	Q	2	Total O 2 2	0	0
19	R	7	Total O 7 7	0	0
19	S	3	Total O 3 3	0	0
19	T	1	Total O 1 1	0	0
19	U	5	Total O 5 5	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
19	V	4	Total 4	O 4	0	0
19	W	7	Total 7	O 7	0	0
19	X	3	Total 3	O 3	0	0
19	Y	9	Total 9	O 9	0	0
19	Z	4	Total 4	O 4	0	0
19	a	11	Total 11	O 11	0	0
19	b	7	Total 7	O 7	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:  97% .




- Molecule 1: Proteasome subunit alpha type-2

Chain O:  95% 5%




- Molecule 2: Proteasome subunit alpha type-3

Chain B:  88% 7% 5%




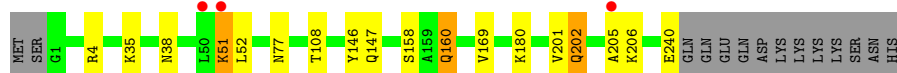
- Molecule 2: Proteasome subunit alpha type-3

Chain P:  88% 6% 5%

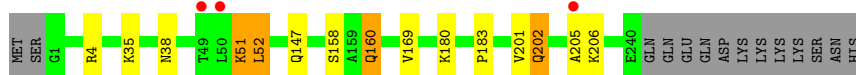
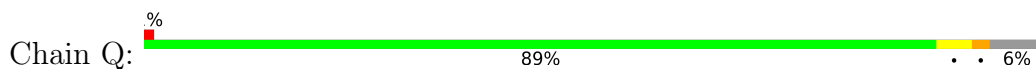


- Molecule 3: Proteasome subunit alpha type-4

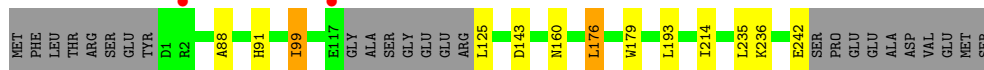
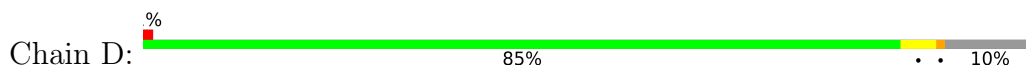
Chain C:  87% 6% 6%



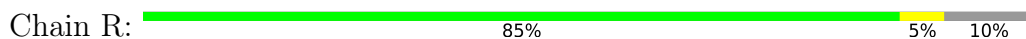
- Molecule 3: Proteasome subunit alpha type-4



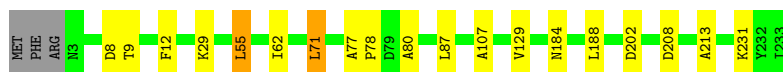
- Molecule 4: Proteasome subunit alpha type-5



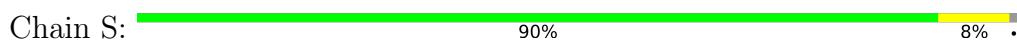
- Molecule 4: Proteasome subunit alpha type-5



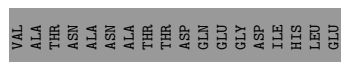
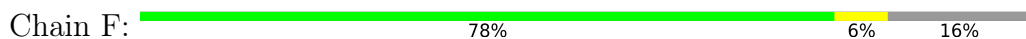
- Molecule 5: Proteasome subunit alpha type-6



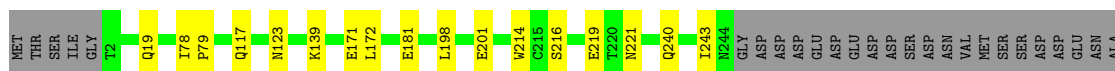
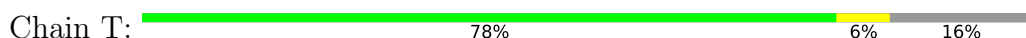
- Molecule 5: Proteasome subunit alpha type-6



- Molecule 6: Probable proteasome subunit alpha type-7




- Molecule 6: Probable proteasome subunit alpha type-7




PRO VAL ALA THR ASN ALA ASN ALA THR ASP GLN GLY ASP ILE HIS LEU GLU

- Molecule 7: Proteasome subunit alpha type-1

Chain G:  90% 6% .


MET SER GLY ALA ALA ALA ALA SER ALA ALA THR ASP GLN GLY ASP ILE HIS LEU GLU

- Molecule 7: Proteasome subunit alpha type-1

Chain U:  89% 6% .


MET SER GLY ALA ALA ALA ALA SER ALA ALA THR ASP GLN GLY ASP ILE HIS LEU GLU

- Molecule 8: Proteasome subunit beta type-2

Chain H:  89% 8% .

T1 T2 I3 N30 C43 A44 V55 T56 I63 L68 P74 L80 K84 D104 P105 I113 T119 V195 R196 E197 E198 E215 E226 GLN VAL ASP ILE THR ALA

- Molecule 8: Proteasome subunit beta type-2

Chain V:  88% 8% . .

T1 T2 I3 N9 N10 T18 N30 A44 V55 L68 L80 K84 D104 P105 I113 T119 L132 E139 E149 S156 S171 M172 L191 R196 E226 GLN VAL ASP ILE THR ALA

- Molecule 9: Proteasome subunit beta type-3

Chain I:  92% 7%

MET S1 G9 I10 V20 S36 N37 K38 K41 P118 F123 C128 A141 L171 D177 D192 R197 D204

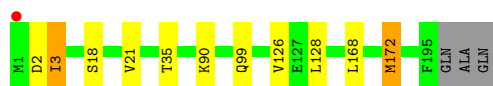
- Molecule 9: Proteasome subunit beta type-3

Chain W:  94% 5%

MET S1 G9 I10 V20 S36 N37 K38 K41 P118 A141 L171 D177 D204

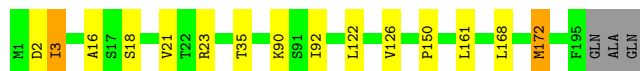
- Molecule 10: Proteasome subunit beta type-4

Chain J:  93% 5% . .



- Molecule 10: Proteasome subunit beta type-4

Chain X: 91% 7% ..



- Molecule 11: Proteasome subunit beta type-5

Chain K: 91% 8% .



- Molecule 11: Proteasome subunit beta type-5

Chain Y: 93% 7%



- Molecule 12: Proteasome subunit beta type-6

Chain L: 95% 5%



- Molecule 12: Proteasome subunit beta type-6

Chain Z: 97% .



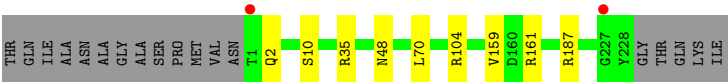
- Molecule 13: Proteasome subunit beta type-7

Chain M: 84% 7% . 9%

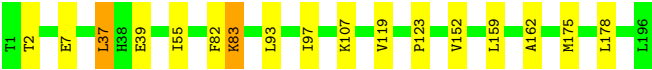
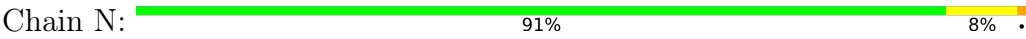


- Molecule 13: Proteasome subunit beta type-7

Chain a: 89% . 7%



● Molecule 14: Proteasome subunit beta type-9,Proteasome subunit beta type-1



● Molecule 14: Proteasome subunit beta type-9,Proteasome subunit beta type-1



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	135.43Å 301.91Å 145.53Å 90.00° 112.83° 90.00°	Depositor
Resolution (Å)	30.00 – 2.85 30.00 – 2.85	Depositor EDS
% Data completeness (in resolution range)	93.9 (30.00-2.85) 93.9 (30.00-2.85)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.28 (at 2.85Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, $R_{free}$	0.183 , 0.227 0.188 , 0.230	Depositor DCC
$R_{free}$ test set	11725 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	56.4	Xtriage
Anisotropy	0.544	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 51.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.52$ , $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	49457	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.67% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  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, MES, CL, 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	0.66	0/1952	0.70	0/2642
1	O	0.67	0/1952	0.70	0/2642
2	B	0.66	0/1934	0.72	0/2618
2	P	0.67	0/1934	0.72	0/2618
3	C	0.67	0/1910	0.72	0/2586
3	Q	0.67	0/1910	0.72	0/2586
4	D	0.67	0/1837	0.71	0/2475
4	R	0.67	0/1837	0.71	0/2475
5	E	0.67	0/1800	0.72	0/2433
5	S	0.67	0/1800	0.72	0/2433
6	F	0.66	0/1932	0.71	0/2609
6	T	0.66	0/1932	0.71	0/2609
7	G	0.65	0/1945	0.70	0/2634
7	U	0.65	0/1945	0.70	0/2634
8	H	0.67	0/1750	0.72	0/2373
8	V	0.67	0/1758	0.72	0/2384
9	I	0.66	0/1611	0.71	0/2174
9	W	0.66	0/1611	0.71	0/2174
10	J	0.65	0/1589	0.71	0/2142
10	X	0.65	0/1589	0.71	0/2142
11	K	0.66	0/1681	0.72	0/2274
11	Y	0.66	0/1681	0.73	0/2274
12	L	0.65	0/1795	0.71	0/2420
12	Z	0.65	0/1795	0.71	0/2420
13	M	0.66	0/1791	0.74	0/2431
13	a	0.66	0/1817	0.74	0/2465
14	N	0.66	0/1531	0.71	0/2073
14	b	0.66	0/1531	0.72	0/2073
All	All	0.66	0/50150	0.72	0/67813

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

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	3	0
1	O	1915	0	1929	5	0
2	B	1904	0	1904	8	0
2	P	1904	0	1904	4	0
3	C	1881	0	1895	6	0
3	Q	1881	0	1895	5	0
4	D	1813	0	1797	4	0
4	R	1813	0	1797	3	0
5	E	1773	0	1775	8	0
5	S	1773	0	1775	7	0
6	F	1892	0	1883	5	0
6	T	1892	0	1883	4	0
7	G	1907	0	1901	5	0
7	U	1907	0	1901	7	0
8	H	1719	0	1719	8	0
8	V	1727	0	1724	23	0
9	I	1581	0	1574	8	0
9	W	1581	0	1574	6	0
10	J	1561	0	1569	5	0
10	X	1561	0	1569	8	0
11	K	1644	0	1595	12	0
11	Y	1644	0	1595	9	0
12	L	1757	0	1711	4	0
12	Z	1757	0	1711	1	0
13	M	1761	0	1765	9	0
13	a	1786	0	1790	0	0
14	N	1502	0	1460	13	0
14	b	1502	0	1460	0	0
15	G	1	0	0	0	0
15	H	1	0	0	0	0
15	I	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	L	1	0	0	0	0
15	U	2	0	0	0	0
15	V	1	0	0	0	0
16	G	1	0	0	0	0
16	I	1	0	0	0	0
16	K	1	0	0	0	0
16	N	1	0	0	0	0
16	U	1	0	0	0	0
16	V	1	0	0	0	0
16	W	1	0	0	0	0
16	Y	1	0	0	0	0
16	Z	1	0	0	0	0
17	M	12	0	13	0	0
17	a	12	0	13	0	0
18	N	5	0	0	0	0
18	b	5	0	0	0	0
19	A	4	0	0	0	0
19	B	8	0	0	0	0
19	C	6	0	0	0	0
19	D	6	0	0	0	0
19	E	6	0	0	0	0
19	F	1	0	0	0	0
19	G	6	0	0	0	0
19	H	5	0	0	0	0
19	I	3	0	0	0	0
19	J	8	0	0	0	0
19	K	13	0	0	0	0
19	L	7	0	0	0	0
19	M	9	0	0	0	0
19	N	2	0	0	0	0
19	O	3	0	0	0	0
19	P	4	0	0	0	0
19	Q	2	0	0	0	0
19	R	7	0	0	0	0
19	S	3	0	0	0	0
19	T	1	0	0	0	0
19	U	5	0	0	0	0
19	V	4	0	0	0	0
19	W	7	0	0	0	0
19	X	3	0	0	0	0
19	Y	9	0	0	0	0
19	Z	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	a	11	0	0	0	0
19	b	7	0	0	0	0
All	All	49457	0	49010	164	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 2.

All (164) 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:161:ARG:HH11	13:M:161:ARG:HG3	1.37	0.89
8:V:18:THR:OG1	8:V:30:ASN:HA	1.76	0.86
10:X:92:ILE:HG21	10:X:122:LEU:HA	1.67	0.76
8:V:80:LEU:HD21	8:V:119:THR:HG21	1.69	0.75
13:M:161:ARG:HH11	13:M:161:ARG:CG	2.01	0.73
8:V:156:SER:OG	8:V:191:LEU:CD1	2.39	0.70
8:V:156:SER:OG	8:V:191:LEU:HD12	1.93	0.68
14:N:2:THR:HG21	14:N:162:ALA:HB3	1.75	0.68
14:N:2:THR:HG22	14:N:159:LEU:CD2	2.24	0.67
8:V:18:THR:CG2	8:V:172:ASN:H	2.07	0.67
14:N:37:LEU:HD22	14:N:37:LEU:N	2.11	0.66
13:M:156:ARG:O	13:M:160:ASP:HB2	1.96	0.65
14:N:2:THR:HG22	14:N:159:LEU:HD22	1.82	0.62
8:V:18:THR:HG21	8:V:172:ASN:HB2	1.85	0.59
8:H:43:CYS:SG	8:H:56:THR:CG2	2.91	0.59
7:G:23:PHE:O	7:G:26:THR:HB	2.03	0.58
14:N:2:THR:HG21	14:N:162:ALA:CB	2.33	0.58
7:U:23:PHE:O	7:U:26:THR:HB	2.03	0.58
2:P:217:LYS:C	2:P:219:ALA:H	2.08	0.57
8:V:18:THR:HG23	8:V:172:ASN:H	1.69	0.56
8:V:18:THR:CG2	8:V:172:ASN:N	2.68	0.56
14:N:37:LEU:N	14:N:37:LEU:CD2	2.70	0.55
9:I:9:GLY:HA3	9:I:41:LYS:HE2	1.89	0.55
2:B:217:LYS:C	2:B:219:ALA:H	2.10	0.54
3:C:160:GLN:HE21	3:C:160:GLN:HA	1.72	0.54
8:H:84:LYS:HA	8:H:113:ILE:HD11	1.90	0.53
3:Q:160:GLN:HE21	3:Q:160:GLN:HA	1.74	0.53
3:Q:51:LYS:O	3:Q:52:LEU:HB2	2.08	0.53
11:K:4:LEU:HD22	11:K:4:LEU:C	2.29	0.53
8:V:80:LEU:CD2	8:V:119:THR:HG21	2.39	0.53
10:X:16:ALA:HB2	10:X:161:LEU:HD21	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Y:4:LEU:C	11:Y:4:LEU:HD22	2.29	0.52
8:V:18:THR:HG21	8:V:172:ASN:CB	2.40	0.52
14:N:152:VAL:HA	14:N:175:MET:HE1	1.91	0.52
14:N:83:LYS:HG3	14:N:119:VAL:CG2	2.39	0.52
12:Z:8:ASN:HA	12:Z:30:ILE:O	2.10	0.51
9:I:10:ILE:HG21	9:I:141:ALA:HB3	1.93	0.51
10:X:168:LEU:O	10:X:172:MET:HB2	2.10	0.51
9:W:9:GLY:HA3	9:W:41:LYS:HE2	1.93	0.51
9:W:10:ILE:HG21	9:W:141:ALA:HB3	1.92	0.51
8:V:18:THR:HG22	8:V:172:ASN:O	2.11	0.51
8:V:172:ASN:HB3	8:V:191:LEU:O	2.10	0.51
14:N:7:GLU:HB2	14:N:123:PRO:O	2.12	0.50
11:K:128:CYS:HB2	11:K:137:TYR:CE2	2.46	0.50
8:V:84:LYS:HA	8:V:113:ILE:HD11	1.92	0.50
10:J:21:VAL:HG11	11:K:122:LEU:HD11	1.93	0.50
10:J:168:LEU:O	10:J:172:MET:HB2	2.11	0.50
8:V:18:THR:HG1	8:V:30:ASN:HA	1.73	0.49
11:K:208:ASN:ND2	10:X:150:PRO:HD3	2.28	0.49
5:S:71:LEU:C	5:S:71:LEU:HD22	2.33	0.49
11:K:128:CYS:HB2	11:K:137:TYR:CZ	2.47	0.49
7:U:78:ILE:N	7:U:79:PRO:CD	2.76	0.48
4:R:160:ASN:HB3	4:R:179:TRP:CE2	2.49	0.48
4:D:160:ASN:HB3	4:D:179:TRP:CE2	2.48	0.48
3:Q:35:LYS:HG2	3:Q:158:SER:O	2.13	0.48
7:G:78:ILE:N	7:G:79:PRO:CD	2.76	0.48
12:L:8:ASN:HA	12:L:30:ILE:O	2.14	0.47
11:Y:128:CYS:HB2	11:Y:137:TYR:CZ	2.50	0.47
8:V:3:ILE:HG21	8:V:44:ALA:HB3	1.97	0.47
3:C:35:LYS:HG2	3:C:158:SER:O	2.14	0.47
4:D:176:LEU:HD22	5:E:55:LEU:CD2	2.44	0.47
2:P:47:ALA:HB1	2:P:64:LYS:HD2	1.97	0.47
5:S:12:PHE:H	6:T:19:GLN:HE22	1.62	0.47
11:Y:20:ALA:HB2	11:Y:31:VAL:HG21	1.97	0.47
13:M:97:ALA:HA	13:M:130:VAL:HG21	1.97	0.47
5:E:71:LEU:HD22	5:E:71:LEU:C	2.36	0.46
13:M:187:ARG:NH1	8:V:139:GLU:OE1	2.43	0.46
10:J:3:ILE:HG23	10:J:18:SER:HB3	1.97	0.46
14:N:55:ILE:HD11	14:N:93:LEU:HD13	1.97	0.46
3:Q:201:VAL:O	3:Q:202:GLN:CB	2.64	0.46
11:Y:128:CYS:HB2	11:Y:137:TYR:CE2	2.49	0.46
2:B:47:ALA:HB1	2:B:64:LYS:HD2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:3:ILE:HG21	8:H:44:ALA:HB3	1.98	0.46
1:A:1:MET:HG3	6:F:122:TYR:CZ	2.51	0.46
2:B:50:LYS:HD3	2:B:50:LYS:HA	1.81	0.46
3:C:201:VAL:O	3:C:202:GLN:CB	2.64	0.45
4:D:88:ALA:HA	4:D:99:ILE:HG21	1.98	0.45
6:F:216:SER:HB3	6:F:219:GLU:HB2	1.97	0.45
1:O:122:THR:HG22	2:P:128:ARG:HH21	1.80	0.45
7:G:73:VAL:HG12	7:G:133:THR:HB	1.98	0.45
6:T:216:SER:HB3	6:T:219:GLU:HB2	1.99	0.45
1:A:64:VAL:HG11	1:A:212:ALA:HB3	1.99	0.45
9:W:36:SER:HB2	10:X:126:VAL:HG11	1.99	0.45
13:M:161:ARG:HG3	13:M:161:ARG:NH1	2.15	0.44
4:R:88:ALA:HA	4:R:99:ILE:HG21	2.00	0.44
5:E:77:ALA:N	5:E:78:PRO:CD	2.81	0.44
11:K:46:ALA:HB3	11:K:98:GLY:O	2.17	0.44
7:U:78:ILE:HG22	7:U:79:PRO:HD3	2.00	0.44
8:V:18:THR:HG23	8:V:171:SER:HB2	1.98	0.44
11:K:20:ALA:HB2	11:K:31:VAL:HG21	1.99	0.44
7:U:73:VAL:HG12	7:U:133:THR:HB	1.99	0.44
11:K:44:THR:O	11:K:99:THR:OG1	2.21	0.43
13:M:165:ILE:HB	13:M:166:PRO:HD3	2.00	0.43
5:S:71:LEU:C	5:S:71:LEU:CD2	2.86	0.43
5:S:175:LEU:HA	5:S:178:PHE:CE2	2.52	0.43
8:V:9[B]:ASN:OD1	8:V:10:ASN:N	2.51	0.43
2:B:114:LEU:HD23	2:B:114:LEU:HA	1.89	0.43
5:S:77:ALA:N	5:S:78:PRO:CD	2.82	0.43
7:U:106:ASP:HB3	7:U:146:TYR:CZ	2.53	0.43
9:W:20:VAL:HG13	9:W:118:PRO:HB3	2.00	0.43
7:G:78:ILE:HG22	7:G:79:PRO:HD3	2.00	0.43
10:X:21:VAL:HG11	11:Y:122:LEU:HD11	2.00	0.43
5:E:12:PHE:H	6:F:19:GLN:HE22	1.67	0.43
1:O:149:GLN:O	1:O:156:TYR:HA	2.19	0.43
8:H:84:LYS:HE2	8:H:119:THR:CG2	2.48	0.43
11:Y:4:LEU:HB3	11:Y:128:CYS:SG	2.59	0.43
6:T:198:LEU:HD12	6:T:243:ILE:HG22	2.01	0.43
9:I:20:VAL:HG13	9:I:118:PRO:HB3	2.00	0.42
8:H:63:ILE:HG23	8:H:74:PRO:HB3	2.01	0.42
8:H:104:ASP:HB2	8:H:105:PRO:HD2	2.00	0.42
12:L:146:ILE:HG22	12:L:150:LEU:HD22	2.01	0.42
8:V:18:THR:HG21	8:V:172:ASN:H	1.79	0.42
8:V:104:ASP:HB2	8:V:105:PRO:HD2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:X:23:ARG:HD3	10:X:23:ARG:HA	1.92	0.42
3:C:51:LYS:O	3:C:52:LEU:HB2	2.19	0.42
14:N:2:THR:HG22	14:N:159:LEU:HD23	1.99	0.42
8:V:18:THR:HG23	8:V:172:ASN:N	2.32	0.42
9:I:141:ALA:HB2	9:I:177:ASP:HB2	2.01	0.42
10:X:3:ILE:HG23	10:X:18:SER:HB3	2.01	0.42
5:E:62:ILE:HG21	5:E:213:ALA:HB2	2.02	0.42
11:Y:4:LEU:HD22	11:Y:4:LEU:O	2.19	0.42
11:Y:6:PHE:HA	11:Y:125:ASP:O	2.20	0.42
1:A:122:THR:HG22	2:B:128:ARG:HH21	1.85	0.42
13:M:96:LEU:O	13:M:100:MET:HG2	2.20	0.42
9:I:123:PHE:HA	9:I:128:CYS:O	2.19	0.42
9:I:38:LYS:NZ	11:Y:209:ASN:O	2.53	0.42
9:I:36:SER:HB2	10:J:126:VAL:HG11	2.01	0.42
14:N:55:ILE:HD11	14:N:93:LEU:CD1	2.50	0.42
9:W:141:ALA:HB2	9:W:177:ASP:HB2	2.02	0.42
6:F:198:LEU:HD12	6:F:243:ILE:HG22	2.01	0.41
1:O:64:VAL:HG11	1:O:212:ALA:HB3	2.02	0.41
7:U:106:ASP:HB3	7:U:146:TYR:CE1	2.55	0.41
7:G:34:LEU:C	7:G:34:LEU:HD23	2.40	0.41
4:R:91:HIS:CD2	4:R:99:ILE:HG22	2.55	0.41
5:E:80:ALA:HB2	5:E:129:VAL:HG21	2.03	0.41
8:H:215:GLU:HG2	9:I:197:ARG:HG2	2.01	0.41
2:B:149:THR:O	2:B:156:TYR:HA	2.21	0.41
5:E:71:LEU:C	5:E:71:LEU:CD2	2.89	0.41
2:B:145:TYR:OH	2:B:217:LYS:N	2.54	0.41
10:J:126:VAL:HG12	10:J:128:LEU:HG	2.03	0.41
3:C:201:VAL:HG13	3:C:202:GLN:N	2.35	0.41
6:F:78:ILE:N	6:F:79:PRO:CD	2.84	0.41
11:K:140:LEU:HD12	11:K:140:LEU:HA	1.88	0.41
12:L:124:SER:O	12:L:131:TYR:HA	2.21	0.41
12:L:189:THR:CG2	8:V:196:ARG:NH1	2.84	0.41
13:M:27:LEU:HB2	13:M:192:SER:HB3	2.03	0.41
3:Q:201:VAL:HG13	3:Q:202:GLN:N	2.36	0.41
6:T:78:ILE:N	6:T:79:PRO:CD	2.83	0.41
7:U:34:LEU:C	7:U:34:LEU:HD23	2.41	0.41
1:O:98:LYS:HE3	1:O:104:TYR:CZ	2.56	0.41
8:V:132:LEU:HD12	8:V:132:LEU:HA	1.88	0.41
11:K:209:ASN:O	9:W:38:LYS:NZ	2.53	0.40
1:O:49:LYS:HG3	1:O:210:GLU:HB2	2.03	0.40
2:P:149:THR:O	2:P:156:TYR:HA	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:4:LEU:C	11:K:4:LEU:CD2	2.89	0.40
5:S:62:ILE:HG21	5:S:213:ALA:HB2	2.03	0.40
4:D:91:HIS:HB3	4:D:99:ILE:CG2	2.51	0.40
14:N:82:PHE:CD1	14:N:97:ILE:HD13	2.56	0.40
5:E:87:LEU:HD21	5:E:107:ALA:HB1	2.02	0.40
8:H:3:ILE:CG2	8:H:44:ALA:HB3	2.51	0.40
2:B:217:LYS:C	2:B:219:ALA:N	2.75	0.40
3:C:108:THR:HG21	3:C:146:TYR:HB3	2.04	0.40
11:K:19:ARG:O	11:K:33:LYS:NZ	2.46	0.40
5:S:127:TYR:O	5:S:148:PRO:CB	2.70	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%)	30	49
1	O	248/250 (99%)	238 (96%)	8 (3%)	2 (1%)	16	32
2	B	242/258 (94%)	234 (97%)	4 (2%)	4 (2%)	7	16
2	P	242/258 (94%)	233 (96%)	5 (2%)	4 (2%)	7	16
3	C	238/254 (94%)	230 (97%)	6 (2%)	2 (1%)	16	32
3	Q	238/254 (94%)	228 (96%)	7 (3%)	3 (1%)	10	22
4	D	231/260 (89%)	226 (98%)	5 (2%)	0	100	100
4	R	231/260 (89%)	227 (98%)	4 (2%)	0	100	100
5	E	229/234 (98%)	221 (96%)	8 (4%)	0	100	100
5	S	229/234 (98%)	222 (97%)	7 (3%)	0	100	100
6	F	241/288 (84%)	236 (98%)	5 (2%)	0	100	100
6	T	241/288 (84%)	236 (98%)	5 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	G	239/252 (95%)	232 (97%)	7 (3%)	0	100	100
7	U	239/252 (95%)	234 (98%)	5 (2%)	0	100	100
8	H	224/232 (97%)	218 (97%)	6 (3%)	0	100	100
8	V	225/232 (97%)	219 (97%)	6 (3%)	0	100	100
9	I	202/205 (98%)	194 (96%)	8 (4%)	0	100	100
9	W	202/205 (98%)	195 (96%)	7 (4%)	0	100	100
10	J	193/198 (98%)	188 (97%)	5 (3%)	0	100	100
10	X	193/198 (98%)	189 (98%)	4 (2%)	0	100	100
11	K	210/212 (99%)	207 (99%)	3 (1%)	0	100	100
11	Y	210/212 (99%)	207 (99%)	3 (1%)	0	100	100
12	L	220/222 (99%)	214 (97%)	6 (3%)	0	100	100
12	Z	220/222 (99%)	215 (98%)	5 (2%)	0	100	100
13	M	223/246 (91%)	216 (97%)	6 (3%)	1 (0%)	30	49
13	a	226/246 (92%)	217 (96%)	9 (4%)	0	100	100
14	N	194/196 (99%)	191 (98%)	3 (2%)	0	100	100
14	b	194/196 (99%)	188 (97%)	6 (3%)	0	100	100
All	All	6272/6614 (95%)	6094 (97%)	161 (3%)	17 (0%)	37	55

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	51	VAL
2	B	221	ASP
3	C	202	GLN
2	P	51	VAL
2	P	221	ASP
3	Q	202	GLN
1	A	2	THR
2	B	218	GLY
2	B	220	ASN
1	O	2	THR
2	P	218	GLY
2	P	220	ASN
3	C	205	ALA
13	M	163	SER
1	O	50	LYS

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Mol	Chain	Res	Type
3	Q	205	ALA
3	Q	183	PRO

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	209/209 (100%)	206 (99%)	3 (1%)	62	82
1	O	209/209 (100%)	206 (99%)	3 (1%)	62	82
2	B	203/216 (94%)	198 (98%)	5 (2%)	42	68
2	P	203/216 (94%)	198 (98%)	5 (2%)	42	68
3	C	212/226 (94%)	202 (95%)	10 (5%)	22	44
3	Q	212/226 (94%)	203 (96%)	9 (4%)	25	48
4	D	194/215 (90%)	185 (95%)	9 (5%)	23	44
4	R	194/215 (90%)	185 (95%)	9 (5%)	23	44
5	E	190/193 (98%)	180 (95%)	10 (5%)	19	38
5	S	190/193 (98%)	179 (94%)	11 (6%)	17	34
6	F	201/239 (84%)	192 (96%)	9 (4%)	23	45
6	T	201/239 (84%)	191 (95%)	10 (5%)	20	40
7	G	206/210 (98%)	197 (96%)	9 (4%)	24	46
7	U	206/210 (98%)	197 (96%)	9 (4%)	24	46
8	H	185/190 (97%)	177 (96%)	8 (4%)	25	47
8	V	186/190 (98%)	179 (96%)	7 (4%)	28	54
9	I	172/173 (99%)	169 (98%)	3 (2%)	56	78
9	W	172/173 (99%)	170 (99%)	2 (1%)	67	84
10	J	173/175 (99%)	167 (96%)	6 (4%)	31	57
10	X	173/175 (99%)	168 (97%)	5 (3%)	37	63
11	K	169/169 (100%)	162 (96%)	7 (4%)	26	50
11	Y	169/169 (100%)	162 (96%)	7 (4%)	26	50

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	L	185/185 (100%)	182 (98%)	3 (2%)	58	79
12	Z	185/185 (100%)	180 (97%)	5 (3%)	40	65
13	M	193/208 (93%)	184 (95%)	9 (5%)	22	44
13	a	195/208 (94%)	186 (95%)	9 (5%)	23	44
14	N	161/161 (100%)	156 (97%)	5 (3%)	35	61
14	b	161/161 (100%)	156 (97%)	5 (3%)	35	61
All	All	5309/5538 (96%)	5117 (96%)	192 (4%)	30	55

All (192) 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	50	LYS
2	B	55	LEU
2	B	79	LEU
2	B	191	LEU
2	B	238	LEU
3	C	4	ARG
3	C	38	ASN
3	C	51	LYS
3	C	77	ASN
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	8	ASP
5	E	9	THR

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Mol	Chain	Res	Type
5	E	29	LYS
5	E	55	LEU
5	E	71	LEU
5	E	184	ASN
5	E	188	LEU
5	E	202	ASP
5	E	208	ASP
5	E	231	LYS
6	F	117	GLN
6	F	123	ASN
6	F	139	LYS
6	F	171	GLU
6	F	172	LEU
6	F	181	GLU
6	F	201	GLU
6	F	214	TRP
6	F	240	GLN
7	G	26	THR
7	G	83	ASN
7	G	115	LEU
7	G	117	GLN
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	55	VAL
8	H	56	THR
8	H	68	LEU
8	H	80	LEU
8	H	195	VAL
8	H	196	ARG
8	H	198	GLU
9	I	37	ASN
9	I	171	LEU
9	I	192	ASP
10	J	2	ASP
10	J	3	ILE
10	J	35	THR
10	J	90	LYS
10	J	99	GLN

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Mol	Chain	Res	Type
10	J	172	MET
11	K	4	LEU
11	K	9	GLN
11	K	104	TYR
11	K	107	LYS
11	K	116	ASP
11	K	140	LEU
11	K	148	LEU
12	L	23	LEU
12	L	31	THR
12	L	130	SER
13	M	2	GLN
13	M	10	SER
13	M	48	ASN
13	M	70	LEU
13	M	104	ARG
13	M	161	ARG
13	M	163	SER
13	M	187	ARG
13	M	220	ASP
14	N	37	LEU
14	N	39	GLU
14	N	83	LYS
14	N	107	LYS
14	N	178	LEU
1	O	122	THR
1	O	157	PHE
1	O	250	LEU
2	P	50	LYS
2	P	79	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	52	LEU
3	Q	147	GLN
3	Q	160	GLN
3	Q	169	VAL
3	Q	180	LYS
3	Q	206	LYS

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Mol	Chain	Res	Type
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	8	ASP
5	S	9	THR
5	S	29	LYS
5	S	55	LEU
5	S	71	LEU
5	S	116	GLN
5	S	184	ASN
5	S	188	LEU
5	S	202	ASP
5	S	208	ASP
5	S	231	LYS
6	T	117	GLN
6	T	123	ASN
6	T	139	LYS
6	T	171	GLU
6	T	172	LEU
6	T	181	GLU
6	T	201	GLU
6	T	214	TRP
6	T	221	ASN
6	T	240	GLN
7	U	26	THR
7	U	83	ASN
7	U	115	LEU
7	U	117	GLN
7	U	122	ARG
7	U	125	MET
7	U	208	GLU
7	U	235	ARG
7	U	236	LEU
8	V	18	THR
8	V	30	ASN
8	V	55	VAL

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Mol	Chain	Res	Type
8	V	68	LEU
8	V	80	LEU
8	V	132	LEU
8	V	149	GLU
9	W	37	ASN
9	W	171	LEU
10	X	2	ASP
10	X	3	ILE
10	X	35	THR
10	X	90	LYS
10	X	172	MET
11	Y	4	LEU
11	Y	9	GLN
11	Y	100	MET
11	Y	104	TYR
11	Y	116	ASP
11	Y	140	LEU
11	Y	148	LEU
12	Z	23	LEU
12	Z	31	THR
12	Z	49	ASN
12	Z	130	SER
12	Z	136	CYS
13	a	2	GLN
13	a	10	SER
13	a	35	ARG
13	a	48	ASN
13	a	70	LEU
13	a	104	ARG
13	a	159	VAL
13	a	161	ARG
13	a	187	ARG
14	b	35	SER
14	b	83	LYS
14	b	132	THR
14	b	178	LEU
14	b	185	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (104) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	20	GLN

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Mol	Chain	Res	Type
2	B	58	GLN
2	B	95	GLN
2	B	119	GLN
2	B	123	GLN
2	B	155	ASN
2	B	176	GLN
3	C	17	GLN
3	C	38	ASN
3	C	77	ASN
3	C	147	GLN
3	C	160	GLN
4	D	15	GLN
4	D	91	HIS
4	D	100	ASN
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	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
6	F	240	GLN
7	G	30	ASN
7	G	83	ASN
7	G	114	ASN
7	G	117	GLN
7	G	121	GLN
7	G	166	GLN
8	H	22	GLN
8	H	30	ASN
8	H	66	HIS
8	H	189	ASN
9	I	37	ASN
10	J	55	GLN
11	K	85	ASN

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Mol	Chain	Res	Type
11	K	176	ASN
11	K	190	ASN
11	K	208	ASN
12	L	3	ASN
12	L	49	ASN
12	L	70	ASN
12	L	158	ASN
13	M	18	ASN
13	M	48	ASN
13	M	102	GLN
13	M	194	ASN
13	M	213	GLN
2	P	20	GLN
2	P	58	GLN
2	P	95	GLN
2	P	119	GLN
2	P	123	GLN
2	P	176	GLN
3	Q	17	GLN
3	Q	38	ASN
3	Q	77	ASN
3	Q	116	GLN
3	Q	120	GLN
3	Q	147	GLN
3	Q	160	GLN
4	R	15	GLN
4	R	91	HIS
4	R	225	ASN
5	S	68	HIS
5	S	92	ASN
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
6	T	240	GLN

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Mol	Chain	Res	Type
7	U	30	ASN
7	U	83	ASN
7	U	114	ASN
7	U	117	GLN
7	U	121	GLN
7	U	166	GLN
8	V	22	GLN
9	W	37	ASN
10	X	55	GLN
11	Y	9	GLN
11	Y	85	ASN
11	Y	176	ASN
11	Y	190	ASN
12	Z	3	ASN
12	Z	49	ASN
12	Z	70	ASN
13	a	18	ASN
13	a	48	ASN
13	a	102	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

Of 20 ligands modelled in this entry, 16 are monoatomic - leaving 4 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	$\# Z  > 2$
17	MES	M	301	-	12,12,12	0.73	0	14,16,16	0.39	0
18	SO4	b	201	-	4,4,4	0.39	0	6,6,6	0.05	0
18	SO4	N	201	-	4,4,4	0.39	0	6,6,6	0.05	0
17	MES	a	301	-	12,12,12	0.73	0	14,16,16	0.44	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	MES	M	301	-	-	0/6/14/14	0/1/1/1
17	MES	a	301	-	-	4/6/14/14	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
17	a	301	MES	C8-C7-N4-C5
17	a	301	MES	C7-C8-S-O3S
17	a	301	MES	C7-C8-S-O1S
17	a	301	MES	C7-C8-S-O2S

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	250/250 (100%)	-0.43	1 (0%) 89 88	50, 63, 91, 127	0
1	O	250/250 (100%)	-0.38	1 (0%) 89 88	52, 70, 104, 137	0
2	B	244/258 (94%)	-0.39	2 (0%) 82 81	49, 66, 101, 146	0
2	P	244/258 (94%)	-0.27	3 (1%) 76 74	50, 70, 107, 143	0
3	C	240/254 (94%)	-0.31	3 (1%) 74 72	53, 71, 121, 134	0
3	Q	240/254 (94%)	-0.16	3 (1%) 74 72	56, 78, 135, 165	0
4	D	235/260 (90%)	-0.27	2 (0%) 81 79	50, 73, 96, 133	0
4	R	235/260 (90%)	-0.41	0 100 100	53, 71, 97, 119	0
5	E	231/234 (98%)	-0.33	0 100 100	55, 74, 97, 124	0
5	S	231/234 (98%)	-0.32	0 100 100	54, 76, 101, 124	0
6	F	243/288 (84%)	-0.42	0 100 100	48, 70, 103, 137	0
6	T	243/288 (84%)	-0.29	0 100 100	52, 74, 113, 130	0
7	G	241/252 (95%)	-0.43	1 (0%) 89 88	46, 63, 91, 127	0
7	U	241/252 (95%)	-0.36	2 (0%) 82 81	53, 67, 94, 122	0
8	H	226/232 (97%)	-0.43	0 100 100	48, 61, 83, 119	0
8	V	226/232 (97%)	-0.41	0 100 100	38, 66, 87, 139	1 (0%)
9	I	204/205 (99%)	-0.56	0 100 100	42, 58, 81, 98	0
9	W	204/205 (99%)	-0.48	0 100 100	48, 61, 83, 102	0
10	J	195/198 (98%)	-0.49	1 (0%) 87 86	47, 60, 81, 114	0
10	X	195/198 (98%)	-0.46	0 100 100	50, 64, 83, 130	0
11	K	212/212 (100%)	-0.45	0 100 100	49, 62, 78, 92	0
11	Y	212/212 (100%)	-0.57	0 100 100	49, 60, 75, 99	0
12	L	222/222 (100%)	-0.42	0 100 100	49, 63, 91, 125	0
12	Z	222/222 (100%)	-0.46	0 100 100	47, 61, 85, 118	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	M	225/246 (91%)	-0.49	1 (0%) 89 88	49, 63, 85, 113	0
13	a	228/246 (92%)	-0.43	2 (0%) 81 79	47, 60, 87, 125	0
14	N	196/196 (100%)	-0.38	0 100 100	51, 63, 87, 111	0
14	b	196/196 (100%)	-0.39	0 100 100	49, 64, 90, 115	0
All	All	6331/6614 (95%)	-0.40	22 (0%) 90 90	38, 66, 100, 165	1 (0%)

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	P	1	GLY	4.5
3	Q	50	LEU	4.2
13	a	1	THR	3.9
7	U	2	GLY	3.8
3	C	50	LEU	3.7
2	P	51	VAL	3.6
3	C	205	ALA	3.4
10	J	1	MET	3.4
3	Q	49	THR	3.0
3	Q	205	ALA	2.9
1	A	2	THR	2.8
13	M	69	ASP	2.8
7	G	242	GLN	2.5
2	B	218	GLY	2.4
2	P	52	THR	2.4
3	C	51	LYS	2.3
4	D	117	GLU	2.3
2	B	222	GLY	2.2
1	O	52	SER	2.2
7	U	242	GLN	2.1
13	a	227	GLY	2.1
4	D	2	ARG	2.1

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

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

## 6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
17	MES	a	301	12/12	0.88	0.17	112,117,123,125	0
17	MES	M	301	12/12	0.89	0.15	116,122,126,128	0
18	SO4	b	201	5/5	0.93	0.12	98,99,106,107	0
18	SO4	N	201	5/5	0.94	0.19	89,90,95,97	0
16	MG	K	301	1/1	0.94	0.08	96,96,96,96	0
16	MG	Z	301	1/1	0.95	0.09	73,73,73,73	0
16	MG	W	301	1/1	0.96	0.17	70,70,70,70	0
16	MG	V	302	1/1	0.97	0.13	89,89,89,89	0
15	CL	V	301	1/1	0.97	0.14	79,79,79,79	0
16	MG	Y	301	1/1	0.97	0.06	61,61,61,61	0
15	CL	L	301	1/1	0.97	0.16	71,71,71,71	0
15	CL	H	301	1/1	0.98	0.14	67,67,67,67	0
16	MG	I	302	1/1	0.98	0.08	66,66,66,66	0
15	CL	U	302	1/1	0.98	0.07	58,58,58,58	0
16	MG	U	303	1/1	0.98	0.05	60,60,60,60	0
16	MG	N	202	1/1	0.99	0.08	63,63,63,63	0
15	CL	G	301	1/1	0.99	0.04	57,57,57,57	0
16	MG	G	302	1/1	0.99	0.03	67,67,67,67	0
15	CL	U	301	1/1	0.99	0.04	57,57,57,57	0
15	CL	I	301	1/1	0.99	0.10	61,61,61,61	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.