



# Full wwPDB X-ray Structure Validation Report ⓘ

Dec 5, 2016 – 03:18 PM EST

PDB ID : 5L67  
Title : Yeast 20S proteasome with mouse beta5i (1-138) and mouse beta6 (97-111; 118-133) in complex with PR-924  
Authors : Groll, M.; Huber, E.M.  
Deposited on : 2016-05-28  
Resolution : 2.60 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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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 : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20028442  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20028442

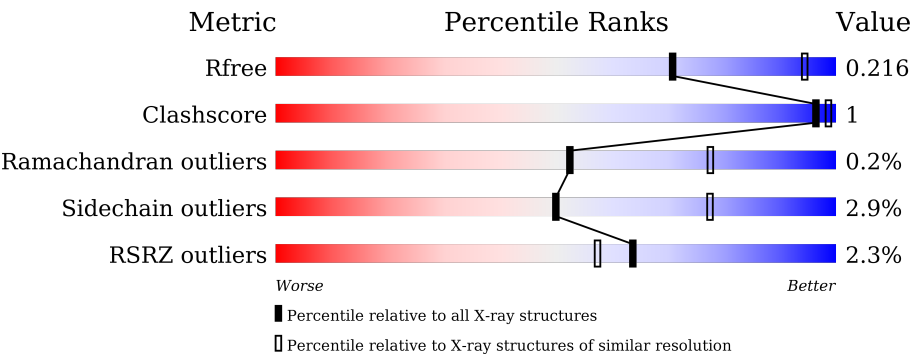
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



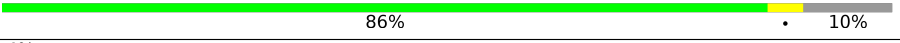

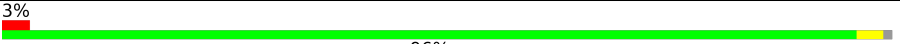
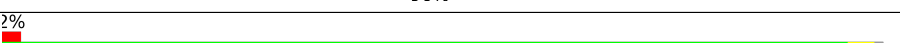
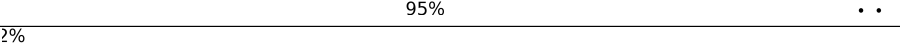
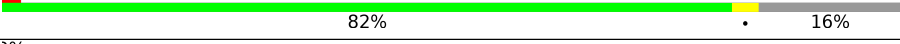



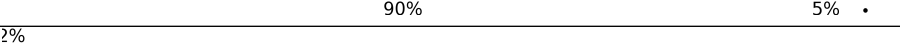



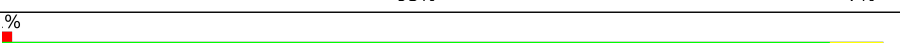
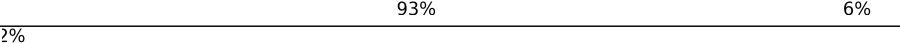
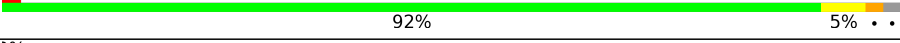



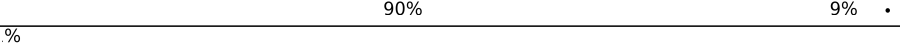
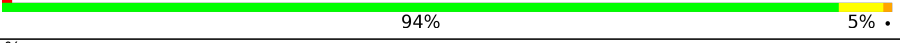
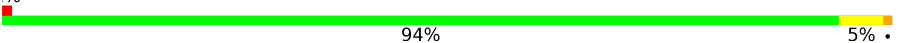
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)

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

Mol	Chain	Length	Quality of chain
1	A	250	<div><div>3%</div><div>98%</div><div>•</div></div>
1	O	250	<div><div>3%</div><div>98%</div><div>•</div></div>
2	B	258	<div><div>3%</div><div>89%</div><div>5% 5%</div></div>
2	P	258	<div><div>3%</div><div>89%</div><div>5% 5%</div></div>
3	C	254	<div><div>6%</div><div>87%</div><div>6% • 6%</div></div>
3	Q	254	<div><div>6%</div><div>87%</div><div>6% • 6%</div></div>

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Mol	Chain	Length	Quality of chain
4	D	260	
4	R	260	
5	E	234	
5	S	234	
6	F	288	
6	T	288	
7	G	252	
7	U	252	
8	H	232	
8	V	232	
9	I	205	
9	W	205	
10	J	198	
10	X	198	
11	K	211	
11	Y	211	
12	L	222	
12	Z	222	
13	M	246	
13	a	246	
14	N	196	
14	b	196	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
15	MG	J	201	-	-	-	X
15	MG	Y	301	-	-	-	X
17	39V	K	301	-	-	-	X
18	MES	K	303	-	-	-	X
18	MES	Y	303	-	-	-	X

## 2 Entry composition

There are 19 unique types of molecules in this entry. The entry contains 50030 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	0	0
			1719	1082	298	332	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-8,Proteasome subunit beta type-5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	211	Total	C	N	O	S	0	0	0
			1645	1039	281	313	12			
11	Y	211	Total	C	N	O	S	0	0	0
			1645	1039	281	313	12			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	233	Total	C	N	O	S	0	1	0
			1832	1159	315	351	7			
13	a	233	Total	C	N	O	S	0	2	0
			1840	1164	318	351	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
			1512	955	250	300	7			
14	b	196	Total	C	N	O	S	0	0	0
			1512	955	250	300	7			

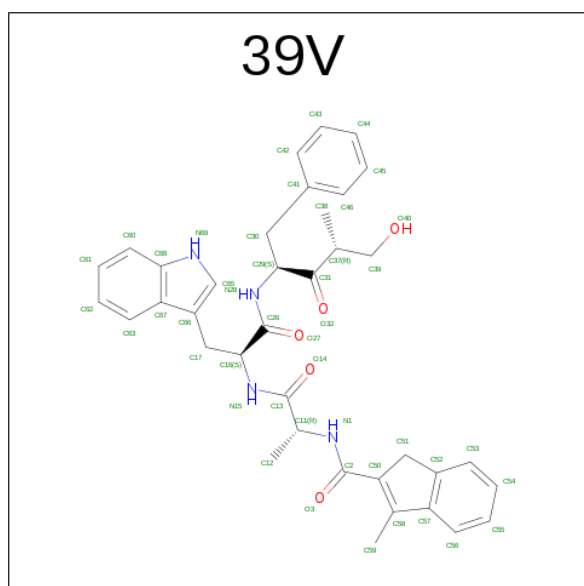
- Molecule 15 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	G	1	Total Mg 1 1	0	0
15	J	1	Total Mg 1 1	0	0
15	K	1	Total Mg 1 1	0	0
15	I	2	Total Mg 2 2	0	0
15	Z	1	Total Mg 1 1	0	0
15	N	1	Total Mg 1 1	0	0
15	Y	1	Total Mg 1 1	0	0
15	L	1	Total Mg 1 1	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	G	1	Total Cl 1 1	0	0
16	U	1	Total Cl 1 1	0	0

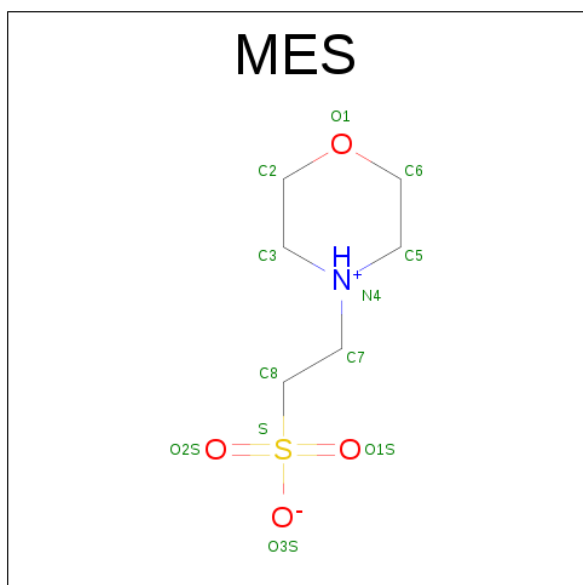
- Molecule 17 is N-[(3-methyl-1H-inden-2-yl)carbonyl]-D-alanyl-N-[(2S,4R)-5-hydroxy-4-methyl-3-oxo-1-phenylpentan-2-yl]-L-tryptophanamide (three-letter code: 39V) (formula: C<sub>37</sub>H<sub>40</sub>N<sub>4</sub>O<sub>5</sub>).





Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
17	K	1	Total	C	N	O	0	0
			46	37	4	5		
17	Y	1	Total	C	N	O	0	0
			46	37	4	5		

- Molecule 18 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: C<sub>6</sub>H<sub>13</sub>NO<sub>4</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
18	K	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
18	Y	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 19 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
19	A	29	Total	O	0	0
			29	29		
19	B	17	Total	O	0	0
			17	17		
19	C	18	Total	O	0	0
			18	18		
19	D	14	Total	O	0	0
			14	14		
19	E	9	Total	O	0	0
			9	9		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
19	F	16	Total O 16 16	0	0
19	G	20	Total O 20 20	0	0
19	H	27	Total O 27 27	0	0
19	I	20	Total O 20 20	0	0
19	J	16	Total O 16 16	0	0
19	K	12	Total O 12 12	0	0
19	L	18	Total O 18 18	0	0
19	M	27	Total O 27 27	0	0
19	N	15	Total O 15 15	0	0
19	O	16	Total O 16 16	0	0
19	P	16	Total O 16 16	0	0
19	Q	6	Total O 6 6	0	0
19	R	16	Total O 16 16	0	0
19	S	12	Total O 12 12	0	0
19	T	10	Total O 10 10	0	0
19	U	23	Total O 23 23	0	0
19	V	26	Total O 26 26	0	0
19	W	17	Total O 17 17	0	0
19	X	15	Total O 15 15	0	0
19	Y	18	Total O 18 18	0	0
19	Z	15	Total O 15 15	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
19	a	28	Total	O	0	0
			28	28		
19	b	21	Total	O	0	0
			21	21		

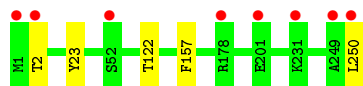
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

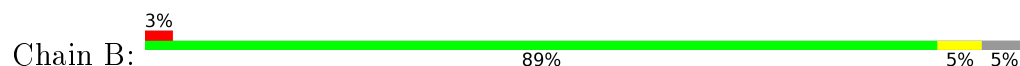
- Molecule 1: Proteasome subunit alpha type-2



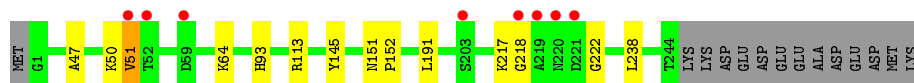
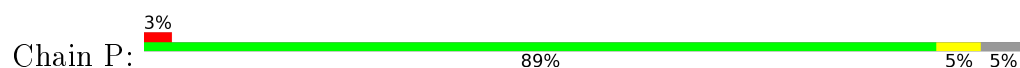
- Molecule 1: Proteasome subunit alpha type-2



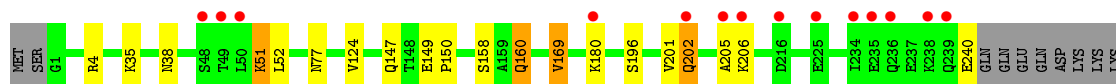
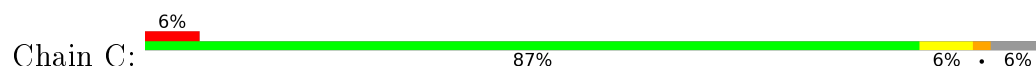
- Molecule 2: Proteasome subunit alpha type-3

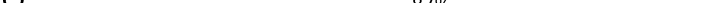


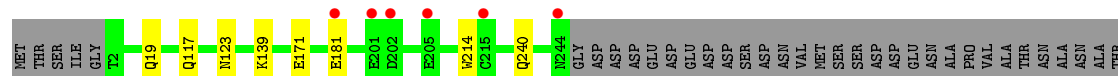
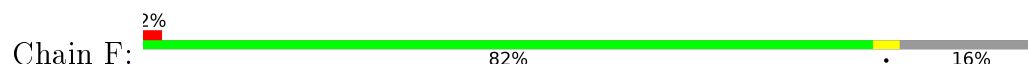
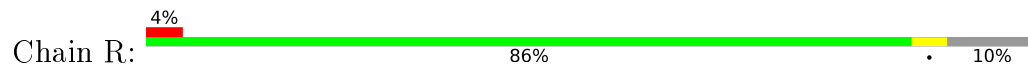
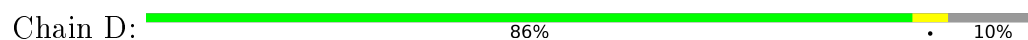
- Molecule 2: Proteasome subunit alpha type-3



- Molecule 3: Proteasome subunit alpha type-4

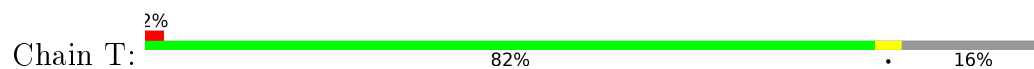


- Chain Q:  6% 87% 6% • 6%



THR  
ASP  
GLN  
GLU  
GLY  
ASP  
ILE  
HIS  
LEU  
GLU

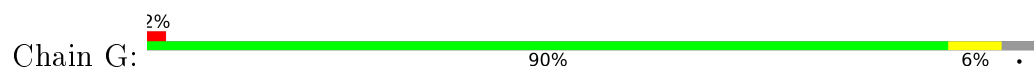
- Molecule 6: Probable proteasome subunit alpha type-7



MET THR SER GLY ALA ALA SER ALA ALA G2 Y3 F23 T26 V73 I78 P79 N83 L115 R122 M125 T133 D149 P150 K179 E208 D222 R235 E241 Q242 ASP

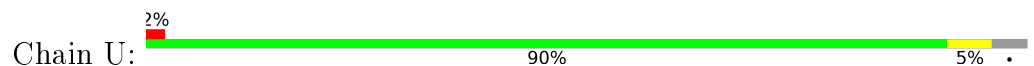
THR  
ASP  
GLN  
GLU  
GLY  
ASP  
ILE  
HIS  
LEU  
GLU

- Molecule 7: Proteasome subunit alpha type-1



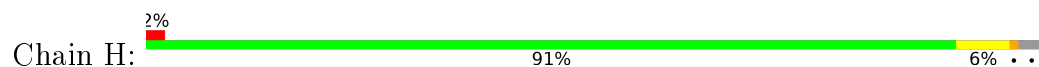
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- Molecule 7: Proteasome subunit alpha type-1



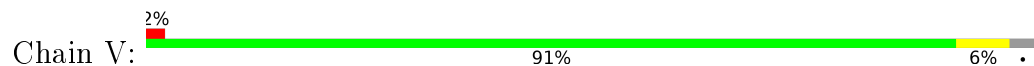
MET SER GLY ALA ALA SER ALA ALA G2 Y3 F23 T26 V73 I78 P79 N83 L115 R122 M125 T133 D149 P150 K179 E208 D222 R235 E241 Q242 ASP

- Molecule 8: Proteasome subunit beta type-2



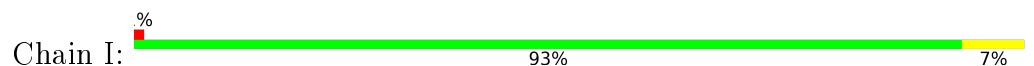
T1 T2 I3 A16 N30 H35 A44 A50 V55 T56 L68 D104 P105 S112 L125 K153 R196 R219 I220 C221 I223 I224 Q225 E226 GLN VAL ASP ILE THR ALA

- Molecule 8: Proteasome subunit beta type-2



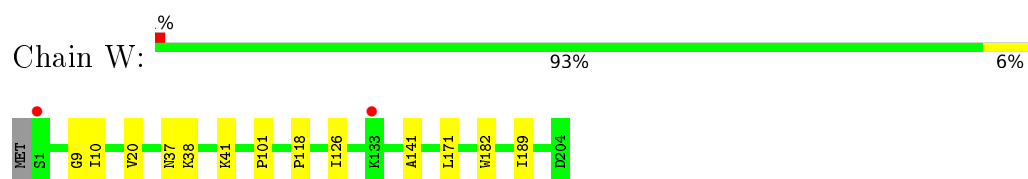
T1 T2 I3 A16 N30 H35 A44 A50 V55 T56 L68 D104 P105 S112 L125 K153 R196 R219 I220 C221 I223 I224 Q225 E226 GLN VAL ASP ILE THR ALA

- Molecule 9: Proteasome subunit beta type-3

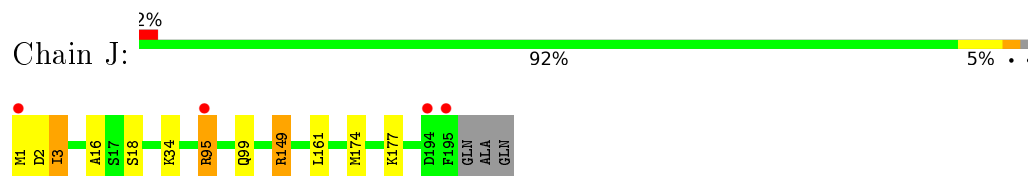


MET S1 G9 I10 V20 N37 K38 K41 P101 P118 P126 K133 A141 E150 L171 W182 I189 D204

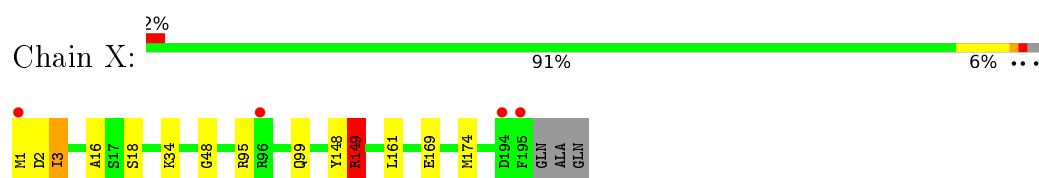
- Molecule 9: Proteasome subunit beta type-3



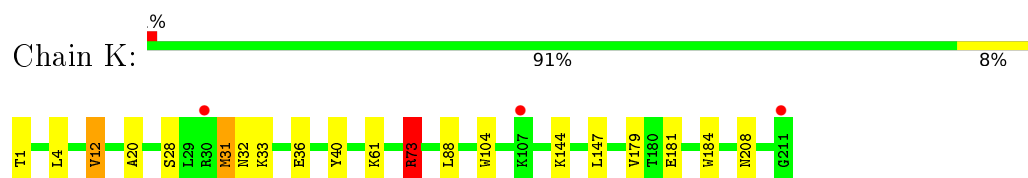
- Molecule 10: Proteasome subunit beta type-4



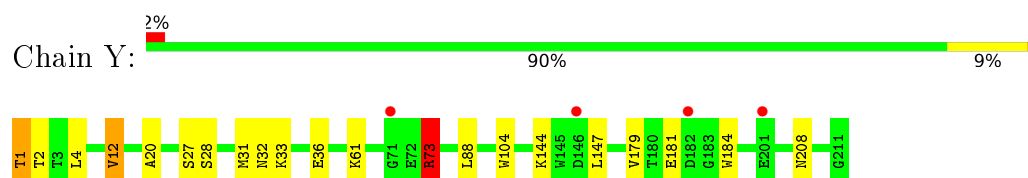
- Molecule 10: Proteasome subunit beta type-4



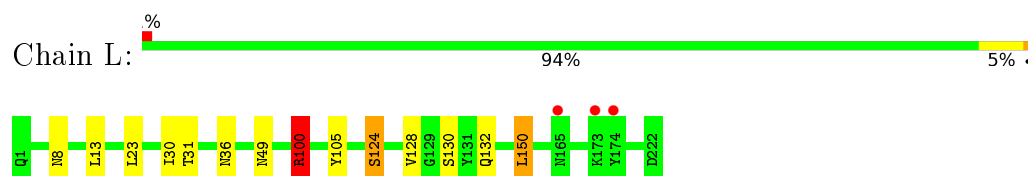
- Molecule 11: Proteasome subunit beta type-8, Proteasome subunit beta type-5



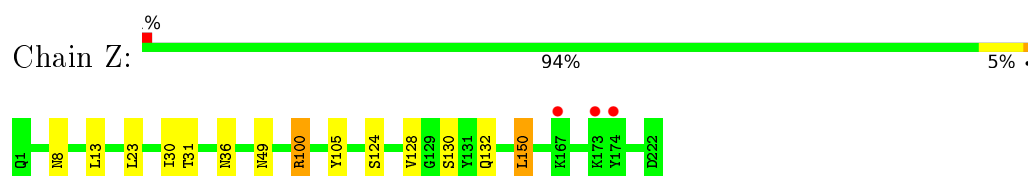
- Molecule 11: Proteasome subunit beta type-8, Proteasome subunit beta type-5




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



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



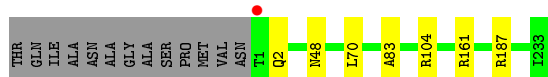
- Molecule 13: Proteasome subunit beta type-7

Chain M:  90% • 5%




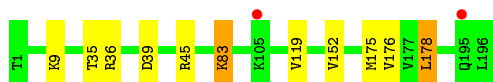
- Molecule 13: Proteasome subunit beta type-7

Chain a:  92% • 5%



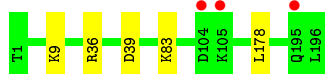
- Molecule 14: Proteasome subunit beta type-1

Chain N:  94% 5% •



- Molecule 14: Proteasome subunit beta type-1

Chain b:  97% 2% •





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	135.56Å 300.68Å 145.63Å 90.00° 112.94° 90.00°	Depositor
Resolution (Å)	15.00 – 2.60 14.99 – 2.60	Depositor EDS
% Data completeness (in resolution range)	98.8 (15.00-2.60) 98.8 (14.99-2.60)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.69 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, $R_{free}$	0.191 , 0.213 0.195 , 0.216	Depositor DCC
$R_{free}$ test set	16111 reflections (5.26%)	DCC
Wilson B-factor (Å <sup>2</sup> )	57.1	Xtriage
Anisotropy	0.100	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 44.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	50030	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.36% of the height of the origin peak. No significant pseudotranslation is detected.*

<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: MG, 39V, MES, CL

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.27	0/1952	0.46	0/2642
1	O	0.27	0/1952	0.46	0/2642
2	B	0.27	0/1934	0.48	0/2618
2	P	0.27	0/1934	0.48	0/2618
3	C	0.27	0/1910	0.49	0/2586
3	Q	0.27	0/1910	0.49	0/2586
4	D	0.27	0/1837	0.46	0/2475
4	R	0.27	0/1837	0.46	0/2475
5	E	0.27	0/1800	0.46	0/2433
5	S	0.27	0/1800	0.46	0/2433
6	F	0.27	0/1932	0.44	0/2609
6	T	0.27	0/1932	0.44	0/2609
7	G	0.27	0/1945	0.46	0/2634
7	U	0.27	0/1945	0.46	0/2634
8	H	0.25	0/1750	0.49	0/2373
8	V	0.25	0/1750	0.49	0/2373
9	I	0.27	0/1611	0.50	0/2174
9	W	0.27	0/1611	0.50	0/2174
10	J	0.27	0/1589	0.96	6/2142 (0.3%)
10	X	0.27	0/1589	0.96	6/2142 (0.3%)
11	K	0.30	0/1681	0.61	4/2268 (0.2%)
11	Y	0.30	0/1681	0.62	6/2268 (0.3%)
12	L	0.28	0/1802	0.77	3/2430 (0.1%)
12	Z	0.28	0/1802	0.76	3/2430 (0.1%)
13	M	0.27	0/1866	0.51	0/2528
13	a	0.27	0/1877	0.50	0/2542
14	N	0.25	0/1541	0.48	0/2087
14	b	0.25	0/1541	0.48	0/2087
All	All	0.27	0/50311	0.55	28/68012 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying

if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
10	J	0	2
10	X	0	1
All	All	0	3

There are no bond length outliers.

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	L	100	ARG	NE-CZ-NH1	-20.30	110.15	120.30
10	X	149	ARG	NE-CZ-NH2	-20.27	110.16	120.30
10	J	95	ARG	NE-CZ-NH2	-20.05	110.28	120.30
12	Z	100	ARG	NE-CZ-NH2	-19.85	110.38	120.30
10	J	149	ARG	NE-CZ-NH1	-19.78	110.41	120.30
10	X	95	ARG	NE-CZ-NH1	-19.71	110.44	120.30
12	L	100	ARG	NE-CZ-NH2	19.35	129.97	120.30
12	Z	100	ARG	NE-CZ-NH1	18.95	129.78	120.30
10	X	95	ARG	NE-CZ-NH2	16.46	128.53	120.30
10	J	149	ARG	NE-CZ-NH2	16.38	128.49	120.30
10	J	95	ARG	NE-CZ-NH1	15.63	128.12	120.30
10	X	149	ARG	NE-CZ-NH1	15.18	127.89	120.30
11	K	73	ARG	CG-CD-NE	10.29	133.41	111.80
10	X	149	ARG	CD-NE-CZ	9.73	137.23	123.60
10	J	149	ARG	CD-NE-CZ	9.60	137.05	123.60
12	Z	100	ARG	CD-NE-CZ	9.59	137.03	123.60
10	J	95	ARG	CD-NE-CZ	9.42	136.78	123.60
11	Y	73	ARG	CG-CD-NE	9.33	131.40	111.80
12	L	100	ARG	CD-NE-CZ	9.23	136.52	123.60
10	X	95	ARG	CD-NE-CZ	9.07	136.30	123.60
11	Y	73	ARG	NE-CZ-NH1	8.12	124.36	120.30
11	K	73	ARG	NE-CZ-NH1	6.63	123.62	120.30
11	K	1	THR	N-CA-C	6.05	127.35	111.00
11	Y	1	THR	CB-CA-C	-5.80	95.94	111.60
11	Y	1	THR	CA-CB-CG2	5.62	120.28	112.40
11	Y	1	THR	N-CA-C	5.48	125.78	111.00
11	Y	73	ARG	CD-NE-CZ	5.27	130.98	123.60
11	K	1	THR	CA-CB-CG2	5.13	119.58	112.40

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
10	J	149	ARG	Sidechain
10	J	95	ARG	Sidechain
10	X	149	ARG	Sidechain

## 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	0	0
1	O	1915	0	1929	1	0
2	B	1904	0	1904	6	0
2	P	1904	0	1904	5	0
3	C	1881	0	1895	8	0
3	Q	1881	0	1895	7	0
4	D	1813	0	1797	4	0
4	R	1813	0	1797	4	0
5	E	1773	0	1775	1	0
5	S	1773	0	1775	2	0
6	F	1892	0	1883	1	0
6	T	1892	0	1883	1	0
7	G	1907	0	1901	4	0
7	U	1907	0	1901	4	0
8	H	1719	0	1719	10	0
8	V	1719	0	1719	6	0
9	I	1581	0	1574	9	0
9	W	1581	0	1574	6	0
10	J	1561	0	1569	4	0
10	X	1561	0	1569	6	0
11	K	1645	0	1589	11	0
11	Y	1645	0	1589	14	0
12	L	1764	0	1716	7	0
12	Z	1764	0	1716	6	0
13	M	1832	0	1845	2	0
13	a	1840	0	1858	0	0
14	N	1512	0	1481	4	0
14	b	1512	0	1481	0	0
15	G	1	0	0	0	0
15	I	2	0	0	0	0
15	J	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	K	1	0	0	0	0
15	L	1	0	0	0	0
15	N	1	0	0	0	0
15	Y	1	0	0	0	0
15	Z	1	0	0	0	0
16	G	1	0	0	0	0
16	U	1	0	0	0	0
17	K	46	0	39	11	0
17	Y	46	0	39	8	0
18	K	12	0	13	2	0
18	Y	12	0	13	0	0
19	A	29	0	0	0	0
19	B	17	0	0	1	0
19	C	18	0	0	0	0
19	D	14	0	0	0	0
19	E	9	0	0	0	0
19	F	16	0	0	0	0
19	G	20	0	0	0	0
19	H	27	0	0	0	0
19	I	20	0	0	0	0
19	J	16	0	0	0	0
19	K	12	0	0	0	0
19	L	18	0	0	0	0
19	M	27	0	0	0	0
19	N	15	0	0	0	0
19	O	16	0	0	0	0
19	P	16	0	0	1	0
19	Q	6	0	0	0	0
19	R	16	0	0	0	0
19	S	12	0	0	0	0
19	T	10	0	0	0	0
19	U	23	0	0	0	0
19	V	26	0	0	0	0
19	W	17	0	0	0	0
19	X	15	0	0	0	0
19	Y	18	0	0	0	0
19	Z	15	0	0	0	0
19	a	28	0	0	0	0
19	b	21	0	0	0	0
All	All	50030	0	49271	132	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 1.

All (132) 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)
17:Y:302:39V:H9	12:Z:124:SER:OG	1.66	0.96
11:Y:73:ARG:HB2	11:Y:73:ARG:HH11	1.48	0.77
17:K:301:39V:H9	12:L:124:SER:OG	1.86	0.75
17:Y:302:39V:H4	17:Y:302:39V:H1	1.54	0.72
11:K:73:ARG:HB2	11:K:73:ARG:HH11	1.59	0.67
12:L:100:ARG:HD2	12:L:105:TYR:CE2	2.33	0.64
17:Y:302:39V:H5	12:Z:130:SER:OG	1.96	0.64
9:I:38:LYS:NZ	11:Y:208:ASN:O	2.31	0.64
17:K:301:39V:H4	17:K:301:39V:H1	1.66	0.61
14:N:152:VAL:HA	14:N:175:MET:HE1	1.83	0.61
11:K:208:ASN:O	9:W:38:LYS:NZ	2.34	0.60
17:Y:302:39V:H4	17:Y:302:39V:N1	2.16	0.57
12:Z:100:ARG:HD3	12:Z:105:TYR:CE2	2.39	0.57
12:L:100:ARG:HD2	12:L:105:TYR:CZ	2.39	0.57
17:K:301:39V:O40	17:K:301:39V:O32	2.22	0.56
10:X:1:MET:HG2	10:X:34:LYS:HE3	1.87	0.56
10:J:1:MET:HG2	10:J:34:LYS:HE3	1.87	0.56
8:V:35:HIS:HB3	8:V:56:THR:HG21	1.89	0.55
17:K:301:39V:H4	17:K:301:39V:N1	2.23	0.54
8:H:35:HIS:HB3	8:H:56:THR:HG21	1.89	0.54
2:B:93:HIS:HB3	19:B:301:HOH:O	2.07	0.53
14:N:83:LYS:HG3	14:N:119:VAL:CG2	2.38	0.53
8:H:3:ILE:HG21	8:H:44:ALA:HB1	1.91	0.51
8:V:3:ILE:HG21	8:V:44:ALA:HB1	1.93	0.51
4:R:89:VAL:HG12	11:Y:61:LYS:HG3	1.93	0.51
11:Y:1:THR:HG22	11:Y:2:THR:N	2.24	0.51
3:C:201:VAL:O	3:C:202:GLN:CB	2.59	0.51
14:N:176:VAL:HG12	14:N:178:LEU:HD13	1.93	0.50
8:H:3:ILE:HG21	8:H:44:ALA:CB	2.42	0.50
17:K:301:39V:H5	12:L:130:SER:OG	2.12	0.50
3:Q:201:VAL:O	3:Q:202:GLN:CB	2.59	0.50
7:U:23:PHE:O	7:U:26:THR:HB	2.11	0.50
7:G:23:PHE:O	7:G:26:THR:HB	2.11	0.49
11:K:36:GLU:OE1	11:K:184:TRP:CH2	2.66	0.49
8:V:3:ILE:HG21	8:V:44:ALA:CB	2.42	0.49
11:Y:36:GLU:OE1	11:Y:184:TRP:CH2	2.65	0.49
17:Y:302:39V:C59	17:Y:302:39V:H1	2.22	0.49
10:X:16:ALA:HB2	10:X:161:LEU:HD21	1.96	0.48
10:J:16:ALA:HB2	10:J:161:LEU:HD21	1.96	0.48
11:Y:27:SER:HB2	17:Y:302:39V:H11	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:201:VAL:O	3:C:202:GLN:HB3	2.14	0.47
12:Z:31:THR:HG23	12:Z:36:ASN:HD21	1.79	0.47
11:Y:1:THR:CG2	11:Y:2:THR:N	2.78	0.47
11:Y:33:LYS:HE2	17:Y:302:39V:C42	2.45	0.47
12:L:31:THR:HG23	12:L:36:ASN:HD21	1.79	0.46
2:P:93:HIS:HB3	19:P:301:HOH:O	2.13	0.46
3:Q:201:VAL:O	3:Q:202:GLN:HB3	2.15	0.46
2:P:50:LYS:O	2:P:51:VAL:C	2.54	0.46
1:O:23:TYR:CD1	7:U:12:PRO:HA	2.51	0.45
9:I:10:ILE:HG21	9:I:141:ALA:HB3	1.98	0.45
9:I:20:VAL:HG23	9:I:189:ILE:HB	1.97	0.45
3:Q:160:GLN:HE21	3:Q:160:GLN:HA	1.82	0.45
9:W:9:GLY:HA3	9:W:41:LYS:HE2	1.99	0.45
9:I:20:VAL:HG13	9:I:118:PRO:HB3	1.97	0.45
9:W:10:ILE:HG21	9:W:141:ALA:HB3	1.98	0.45
9:W:20:VAL:HG13	9:W:118:PRO:HB3	1.97	0.45
11:K:33:LYS:HE2	17:K:301:39V:C42	2.47	0.45
3:C:160:GLN:HA	3:C:160:GLN:HE21	1.81	0.45
9:I:101:PRO:HB3	9:I:126:ILE:HD12	1.98	0.45
2:B:50:LYS:O	2:B:51:VAL:C	2.55	0.45
12:Z:13:LEU:HD11	12:Z:150:LEU:HD21	1.99	0.44
9:W:20:VAL:HG23	9:W:189:ILE:HB	1.97	0.44
9:W:101:PRO:HB3	9:W:126:ILE:HD12	1.98	0.44
9:I:9:GLY:HA3	9:I:41:LYS:HE2	1.99	0.44
11:Y:104:TRP:CE2	11:Y:181:GLU:HB3	2.52	0.44
4:D:89:VAL:HG12	11:K:61:LYS:HG3	2.00	0.44
11:K:104:TRP:CE2	11:K:181:GLU:HB3	2.52	0.44
3:C:51:LYS:O	3:C:52:LEU:HB2	2.18	0.44
14:N:35:THR:HG21	14:N:45:ARG:HE	1.83	0.44
12:Z:8:ASN:HA	12:Z:30:ILE:O	2.18	0.43
17:K:301:39V:O40	18:K:303:MES:O3S	2.35	0.43
12:L:8:ASN:HA	12:L:30:ILE:O	2.18	0.43
11:K:40:TYR:CD2	11:K:73:ARG:NE	2.86	0.43
2:B:47:ALA:HB1	2:B:64:LYS:HD2	2.01	0.43
12:L:13:LEU:HD11	12:L:150:LEU:HD21	1.99	0.43
3:Q:51:LYS:O	3:Q:52:LEU:HB2	2.18	0.43
11:Y:73:ARG:CB	11:Y:73:ARG:HH11	2.26	0.43
11:K:20:ALA:HB3	11:K:28:SER:HB3	2.00	0.43
10:X:148:TYR:O	10:X:149:ARG:HD3	2.18	0.43
11:Y:144:LYS:HB2	11:Y:147:LEU:HD13	2.01	0.43
11:Y:20:ALA:HB3	11:Y:28:SER:HB3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:78:ILE:N	7:G:79:PRO:CD	2.82	0.43
11:K:31:MET:CE	17:K:301:39V:H7	2.49	0.43
2:P:47:ALA:HB1	2:P:64:LYS:HD2	2.01	0.43
10:J:3:ILE:HG23	10:J:18:SER:HB3	2.01	0.43
17:K:301:39V:N15	17:K:301:39V:C65	2.81	0.43
5:S:12:PHE:H	6:T:19:GLN:HE22	1.67	0.43
17:Y:302:39V:N15	17:Y:302:39V:C65	2.82	0.42
10:X:3:ILE:HG23	10:X:18:SER:HB3	2.01	0.42
2:B:151:ASN:HB2	2:B:152:PRO:CD	2.49	0.42
3:C:169:VAL:HG23	3:C:196:SER:HB2	2.01	0.42
17:K:301:39V:C59	17:K:301:39V:H1	2.28	0.42
11:K:144:LYS:HB2	11:K:147:LEU:HD13	2.01	0.42
11:Y:12:VAL:HG13	11:Y:179:VAL:HB	2.01	0.42
4:D:91:HIS:HB3	4:D:99:ILE:CG2	2.50	0.42
8:H:104:ASP:HB2	8:H:105:PRO:HD2	2.02	0.42
11:K:12:VAL:HG13	11:K:179:VAL:HB	2.01	0.42
2:P:151:ASN:HB2	2:P:152:PRO:CD	2.49	0.42
3:Q:149:GLU:HB2	3:Q:150:PRO:HD2	2.01	0.42
3:Q:169:VAL:HG23	3:Q:196:SER:HB2	2.01	0.42
2:B:124:HIS:HB3	3:C:124:VAL:HG12	2.02	0.42
4:D:160:ASN:HB3	4:D:179:TRP:CE2	2.55	0.42
7:U:78:ILE:N	7:U:79:PRO:CD	2.82	0.42
3:C:149:GLU:HB2	3:C:150:PRO:HD2	2.02	0.42
4:R:160:ASN:HB3	4:R:179:TRP:CE2	2.55	0.42
5:E:12:PHE:H	6:F:19:GLN:HE22	1.68	0.41
3:Q:35:LYS:HG2	3:Q:158:SER:O	2.20	0.41
7:G:149:ASP:HB2	7:G:150:PRO:CD	2.50	0.41
8:H:112:SER:HB3	8:H:125:LEU:HD13	2.02	0.41
10:J:177:LYS:NZ	10:X:169:GLU:O	2.53	0.41
7:U:149:ASP:HB2	7:U:150:PRO:CD	2.51	0.41
8:V:104:ASP:HB2	8:V:105:PRO:HD2	2.02	0.41
8:V:112:SER:HB3	8:V:125:LEU:HD13	2.02	0.41
4:D:91:HIS:CD2	4:D:99:ILE:HG22	2.56	0.41
2:B:145:TYR:OH	2:B:217:LYS:N	2.54	0.41
2:P:145:TYR:OH	2:P:217:LYS:N	2.54	0.41
8:H:196:ARG:NH2	9:I:150:GLU:O	2.54	0.41
11:Y:36:GLU:OE1	11:Y:184:TRP:CZ2	2.74	0.41
3:C:35:LYS:HG2	3:C:158:SER:O	2.20	0.41
8:H:3:ILE:HG23	8:H:16:ALA:HB2	2.02	0.41
4:R:91:HIS:CD2	4:R:99:ILE:HG22	2.56	0.41
17:K:301:39V:O40	18:K:303:MES:S	2.79	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:91:HIS:HB3	4:R:99:ILE:CG2	2.51	0.41
8:H:50:ALA:CB	9:I:126:ILE:HG23	2.51	0.40
13:M:96:LEU:O	13:M:100:MET:HG2	2.22	0.40
8:H:196:ARG:NH2	9:I:150:GLU:HG3	2.36	0.40
5:S:77:ALA:N	5:S:78:PRO:CD	2.85	0.40
10:X:1:MET:N	10:X:48:GLY:O	2.54	0.40
7:G:73:VAL:HG12	7:G:133:THR:HB	2.03	0.40
8:H:3:ILE:HG21	8:H:3:ILE:HD13	1.92	0.40
13:M:127:LEU:HG	13:M:142:LEU:HD12	2.03	0.40
8:V:3:ILE:HG23	8:V:16:ALA:HB2	2.03	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%)	39	65
1	O	248/250 (99%)	239 (96%)	8 (3%)	1 (0%)	39	65
2	B	242/258 (94%)	235 (97%)	4 (2%)	3 (1%)	16	33
2	P	242/258 (94%)	234 (97%)	5 (2%)	3 (1%)	16	33
3	C	238/254 (94%)	233 (98%)	3 (1%)	2 (1%)	24	46
3	Q	238/254 (94%)	233 (98%)	3 (1%)	2 (1%)	24	46
4	D	231/260 (89%)	228 (99%)	3 (1%)	0	100	100
4	R	231/260 (89%)	228 (99%)	3 (1%)	0	100	100
5	E	229/234 (98%)	224 (98%)	5 (2%)	0	100	100
5	S	229/234 (98%)	224 (98%)	5 (2%)	0	100	100
6	F	241/288 (84%)	239 (99%)	2 (1%)	0	100	100
6	T	241/288 (84%)	239 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	G	239/252 (95%)	237 (99%)	2 (1%)	0	100	100
7	U	239/252 (95%)	237 (99%)	2 (1%)	0	100	100
8	H	224/232 (97%)	218 (97%)	6 (3%)	0	100	100
8	V	224/232 (97%)	218 (97%)	6 (3%)	0	100	100
9	I	202/205 (98%)	194 (96%)	8 (4%)	0	100	100
9	W	202/205 (98%)	194 (96%)	8 (4%)	0	100	100
10	J	193/198 (98%)	190 (98%)	3 (2%)	0	100	100
10	X	193/198 (98%)	190 (98%)	3 (2%)	0	100	100
11	K	209/211 (99%)	202 (97%)	7 (3%)	0	100	100
11	Y	209/211 (99%)	202 (97%)	7 (3%)	0	100	100
12	L	220/222 (99%)	216 (98%)	4 (2%)	0	100	100
12	Z	220/222 (99%)	216 (98%)	4 (2%)	0	100	100
13	M	232/246 (94%)	224 (97%)	7 (3%)	1 (0%)	39	65
13	a	233/246 (95%)	225 (97%)	7 (3%)	1 (0%)	39	65
14	N	194/196 (99%)	188 (97%)	6 (3%)	0	100	100
14	b	194/196 (99%)	189 (97%)	5 (3%)	0	100	100
All	All	6285/6612 (95%)	6135 (98%)	136 (2%)	14 (0%)	52	77

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	51	VAL
3	C	202	GLN
2	P	51	VAL
3	Q	202	GLN
1	A	2	THR
2	B	218	GLY
2	B	222	GLY
1	O	2	THR
2	P	218	GLY
2	P	222	GLY
3	C	205	ALA
3	Q	205	ALA
13	a	83	ALA
13	M	83	ALA

### 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%)	74	90
1	O	209/209 (100%)	206 (99%)	3 (1%)	74	90
2	B	203/216 (94%)	200 (98%)	3 (2%)	72	90
2	P	203/216 (94%)	200 (98%)	3 (2%)	72	90
3	C	212/226 (94%)	202 (95%)	10 (5%)	32	59
3	Q	212/226 (94%)	202 (95%)	10 (5%)	32	59
4	D	194/215 (90%)	186 (96%)	8 (4%)	37	66
4	R	194/215 (90%)	186 (96%)	8 (4%)	37	66
5	E	190/193 (98%)	185 (97%)	5 (3%)	54	80
5	S	190/193 (98%)	185 (97%)	5 (3%)	54	80
6	F	201/239 (84%)	194 (96%)	7 (4%)	43	71
6	T	201/239 (84%)	194 (96%)	7 (4%)	43	71
7	G	206/210 (98%)	200 (97%)	6 (3%)	50	77
7	U	206/210 (98%)	200 (97%)	6 (3%)	50	77
8	H	185/190 (97%)	179 (97%)	6 (3%)	46	74
8	V	185/190 (97%)	179 (97%)	6 (3%)	46	74
9	I	172/173 (99%)	169 (98%)	3 (2%)	68	88
9	W	172/173 (99%)	169 (98%)	3 (2%)	68	88
10	J	173/175 (99%)	169 (98%)	4 (2%)	58	83
10	X	173/175 (99%)	169 (98%)	4 (2%)	58	83
11	K	172/172 (100%)	166 (96%)	6 (4%)	43	71
11	Y	172/172 (100%)	166 (96%)	6 (4%)	43	71
12	L	186/186 (100%)	179 (96%)	7 (4%)	40	68
12	Z	186/186 (100%)	181 (97%)	5 (3%)	52	79
13	M	200/208 (96%)	194 (97%)	6 (3%)	48	76
13	a	201/208 (97%)	195 (97%)	6 (3%)	48	76

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	N	162/162 (100%)	157 (97%)	5 (3%)	47	76
14	b	162/162 (100%)	157 (97%)	5 (3%)	47	76
All	All	5331/5548 (96%)	5175 (97%)	156 (3%)	50	77

All (156) 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	113	ARG
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	235	LEU
4	D	236	LYS
4	D	242	GLU
5	E	9	THR
5	E	29	LYS
5	E	71	LEU
5	E	184	ASN
5	E	188	LEU
6	F	117	GLN
6	F	123	ASN
6	F	139	LYS
6	F	171	GLU
6	F	181	GLU

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Mol	Chain	Res	Type
6	F	214	TRP
6	F	240	GLN
7	G	83	ASN
7	G	115	LEU
7	G	122	ARG
7	G	125	MET
7	G	208	GLU
7	G	235	ARG
8	H	3	ILE
8	H	30	ASN
8	H	55	VAL
8	H	68	LEU
8	H	153	LYS
8	H	196	ARG
9	I	37	ASN
9	I	171	LEU
9	I	182	TRP
10	J	2	ASP
10	J	3	ILE
10	J	99	GLN
10	J	174	MET
11	K	4	LEU
11	K	12	VAL
11	K	31	MET
11	K	32	ASN
11	K	73	ARG
11	K	88	LEU
12	L	23	LEU
12	L	49	ASN
12	L	100	ARG
12	L	124	SER
12	L	128	VAL
12	L	132	GLN
12	L	150	LEU
13	M	2	GLN
13	M	48	ASN
13	M	70	LEU
13	M	104	ARG
13	M	161	ARG
13	M	187	ARG
14	N	9	LYS
14	N	36	ARG

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Mol	Chain	Res	Type
14	N	39	ASP
14	N	83	LYS
14	N	178	LEU
1	O	122	THR
1	O	157	PHE
1	O	250	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	77	ASN
3	Q	147	GLN
3	Q	160	GLN
3	Q	169	VAL
3	Q	180	LYS
3	Q	206	LYS
3	Q	240	GLU
4	R	99	ILE
4	R	125	LEU
4	R	143	ASP
4	R	176	LEU
4	R	193	LEU
4	R	235	LEU
4	R	236	LYS
4	R	242	GLU
5	S	9	THR
5	S	29	LYS
5	S	71	LEU
5	S	184	ASN
5	S	188	LEU
6	T	117	GLN
6	T	123	ASN
6	T	139	LYS
6	T	171	GLU
6	T	181	GLU
6	T	214	TRP
6	T	240	GLN
7	U	83	ASN
7	U	115	LEU
7	U	122	ARG

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Mol	Chain	Res	Type
7	U	125	MET
7	U	208	GLU
7	U	235	ARG
8	V	3	ILE
8	V	30	ASN
8	V	55	VAL
8	V	68	LEU
8	V	153	LYS
8	V	196	ARG
9	W	37	ASN
9	W	171	LEU
9	W	182	TRP
10	X	2	ASP
10	X	3	ILE
10	X	99	GLN
10	X	174	MET
11	Y	4	LEU
11	Y	12	VAL
11	Y	31	MET
11	Y	32	ASN
11	Y	73	ARG
11	Y	88	LEU
12	Z	23	LEU
12	Z	49	ASN
12	Z	128	VAL
12	Z	132	GLN
12	Z	150	LEU
13	a	2	GLN
13	a	48	ASN
13	a	70	LEU
13	a	104	ARG
13	a	161	ARG
13	a	187	ARG
14	b	9	LYS
14	b	36	ARG
14	b	39	ASP
14	b	83	LYS
14	b	178	LEU

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

Mol	Chain	Res	Type
1	A	94	HIS
2	B	20	GLN
2	B	58	GLN
2	B	95	GLN
2	B	119	GLN
2	B	123	GLN
3	C	77	ASN
3	C	116	GLN
3	C	120	GLN
3	C	147	GLN
3	C	160	GLN
4	D	15	GLN
4	D	91	HIS
4	D	225	ASN
5	E	68	HIS
5	E	92	ASN
5	E	99	ASN
5	E	116	GLN
5	E	118	ASN
5	E	120	GLN
5	E	151	ASN
5	E	184	ASN
6	F	19	GLN
6	F	86	ASN
6	F	117	GLN
6	F	123	ASN
6	F	191	GLN
7	G	83	ASN
7	G	114	ASN
7	G	117	GLN
7	G	121	GLN
7	G	166	GLN
8	H	66	HIS
9	I	37	ASN
11	K	32	ASN
11	K	175	ASN
12	L	3	ASN
12	L	49	ASN
12	L	70	ASN
12	L	79	HIS
12	L	109	ASN
13	M	48	ASN
13	M	102	GLN

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Mol	Chain	Res	Type
13	M	179	ASN
13	M	194	ASN
13	M	213	GLN
14	N	161	GLN
1	O	94	HIS
2	P	20	GLN
2	P	58	GLN
2	P	95	GLN
2	P	119	GLN
2	P	123	GLN
3	Q	77	ASN
3	Q	116	GLN
3	Q	120	GLN
3	Q	147	GLN
3	Q	160	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
7	U	83	ASN
7	U	114	ASN
7	U	117	GLN
7	U	121	GLN
7	U	166	GLN
9	W	37	ASN
11	Y	32	ASN
11	Y	175	ASN
12	Z	3	ASN
12	Z	49	ASN
12	Z	70	ASN
12	Z	109	ASN

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Mol	Chain	Res	Type
12	Z	158	ASN
13	a	48	ASN
13	a	102	GLN
13	a	194	ASN
13	a	213	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 15 ligands modelled in this entry, 11 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	39V	K	301	11	47,50,50	3.61	15 (31%)	52,70,70	1.43	8 (15%)
18	MES	K	303	-	12,12,12	2.22	1 (8%)	15,16,16	1.94	3 (20%)
17	39V	Y	302	11	47,50,50	3.70	15 (31%)	52,70,70	1.39	7 (13%)
18	MES	Y	303	-	12,12,12	2.16	1 (8%)	15,16,16	1.80	3 (20%)

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	39V	K	301	11	-	0/40/54/54	0/5/5/5
18	MES	K	303	-	-	0/6/14/14	0/1/1/1
17	39V	Y	302	11	-	0/40/54/54	0/5/5/5
18	MES	Y	303	-	-	0/6/14/14	0/1/1/1

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	K	301	39V	C51-C50	-11.35	1.36	1.52
17	Y	302	39V	C51-C50	-11.16	1.37	1.52
17	Y	302	39V	C2-C50	-10.44	1.32	1.49
17	K	301	39V	C2-C50	-9.93	1.33	1.49
18	K	303	MES	C8-S	-7.53	1.66	1.77
17	Y	302	39V	C51-C52	-7.27	1.38	1.50
18	Y	303	MES	C8-S	-7.26	1.66	1.77
17	K	301	39V	C51-C52	-7.11	1.38	1.50
17	K	301	39V	C57-C58	-6.40	1.31	1.44
17	Y	302	39V	C57-C58	-6.11	1.31	1.44
17	K	301	39V	C57-C52	-5.56	1.32	1.39
17	Y	302	39V	C57-C52	-5.29	1.32	1.39
17	K	301	39V	C60-C68	-5.24	1.32	1.41
17	Y	302	39V	C60-C68	-5.24	1.32	1.41
17	Y	302	39V	C63-C67	-5.18	1.31	1.42
17	K	301	39V	C63-C67	-5.16	1.31	1.42
17	K	301	39V	C56-C57	-4.72	1.32	1.39
17	Y	302	39V	C30-C41	-4.66	1.39	1.51
17	K	301	39V	C30-C41	-4.62	1.39	1.51
17	Y	302	39V	C56-C57	-4.45	1.32	1.39
17	K	301	39V	C53-C52	-4.35	1.32	1.39
17	Y	302	39V	C67-C68	-4.17	1.31	1.42
17	Y	302	39V	C53-C52	-4.15	1.32	1.39
17	K	301	39V	C67-C68	-3.85	1.32	1.42
17	Y	302	39V	C65-N69	-2.28	1.31	1.36
17	Y	302	39V	C50-C58	-2.19	1.31	1.36
17	K	301	39V	C65-C66	-2.10	1.31	1.37
17	K	301	39V	C65-N69	-2.10	1.32	1.36
17	K	301	39V	C68-N69	-2.09	1.32	1.38
17	Y	302	39V	C68-N69	-2.02	1.32	1.38
17	K	301	39V	O32-C31	10.02	1.38	1.21
17	Y	302	39V	O32-C31	11.27	1.40	1.21

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	K	301	39V	O32-C31-C37	-4.93	110.54	120.79
17	Y	302	39V	O32-C31-C37	-4.23	112.01	120.79
17	K	301	39V	C30-C29-N28	-3.95	102.44	110.81
17	Y	302	39V	C30-C29-N28	-3.69	102.99	110.81
17	Y	302	39V	C17-C66-C65	-2.88	124.41	127.97
18	K	303	MES	O2S-S-O1S	-2.48	106.96	113.96
17	K	301	39V	C52-C57-C58	-2.40	107.75	109.51
17	Y	302	39V	C62-C61-C60	-2.35	117.05	120.45
17	K	301	39V	C17-C66-C65	-2.35	125.06	127.97
17	Y	302	39V	C52-C57-C58	-2.24	107.86	109.51
17	Y	302	39V	C12-C11-N1	-2.14	106.19	110.27
17	K	301	39V	C12-C11-N1	-2.12	106.23	110.27
17	K	301	39V	C59-C58-C57	-2.07	121.00	124.84
17	K	301	39V	C17-C16-N15	-2.06	106.45	110.81
18	Y	303	MES	O3S-S-C8	2.19	109.55	104.99
17	K	301	39V	C52-C51-C50	2.21	104.58	102.83
17	Y	302	39V	C52-C51-C50	2.30	104.65	102.83
18	K	303	MES	O3S-S-C8	2.71	110.61	104.99
18	Y	303	MES	O2S-S-C8	3.61	109.42	106.87
18	Y	303	MES	O1S-S-C8	4.70	110.19	106.87
18	K	303	MES	O1S-S-C8	6.01	111.11	106.87

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	K	301	39V	11	0
18	K	303	MES	2	0
17	Y	302	39V	8	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	7 (2%) 56 49	36, 54, 89, 125	0
1	O	250/250 (100%)	-0.38	8 (3%) 51 44	41, 58, 102, 135	0
2	B	244/258 (94%)	-0.29	7 (2%) 55 48	40, 60, 102, 157	0
2	P	244/258 (94%)	-0.28	8 (3%) 50 43	43, 63, 106, 155	0
3	C	240/254 (94%)	-0.06	14 (5%) 26 20	39, 65, 134, 168	0
3	Q	240/254 (94%)	0.04	16 (6%) 21 15	29, 74, 157, 197	0
4	D	235/260 (90%)	-0.36	1 (0%) 93 91	44, 63, 95, 130	0
4	R	235/260 (90%)	-0.20	11 (4%) 35 28	53, 71, 112, 143	0
5	E	231/234 (98%)	-0.27	6 (2%) 59 53	46, 64, 102, 144	0
5	S	231/234 (98%)	-0.28	5 (2%) 65 59	49, 70, 109, 141	0
6	F	243/288 (84%)	-0.41	6 (2%) 61 54	40, 60, 108, 136	0
6	T	243/288 (84%)	-0.35	7 (2%) 55 48	38, 66, 120, 154	0
7	G	241/252 (95%)	-0.47	5 (2%) 67 61	38, 55, 92, 150	0
7	U	241/252 (95%)	-0.42	4 (1%) 73 68	41, 55, 90, 130	0
8	H	226/232 (97%)	-0.44	5 (2%) 65 59	39, 53, 86, 145	0
8	V	226/232 (97%)	-0.40	5 (2%) 65 59	40, 55, 87, 163	0
9	I	204/205 (99%)	-0.64	2 (0%) 84 81	38, 53, 85, 105	0
9	W	204/205 (99%)	-0.65	2 (0%) 84 81	40, 54, 84, 109	0
10	J	195/198 (98%)	-0.43	4 (2%) 67 61	38, 56, 81, 124	0
10	X	195/198 (98%)	-0.44	4 (2%) 67 61	41, 57, 84, 134	0
11	K	211/211 (100%)	-0.39	3 (1%) 78 74	46, 62, 93, 118	0
11	Y	211/211 (100%)	-0.40	4 (1%) 70 64	45, 63, 93, 122	0
12	L	222/222 (100%)	-0.41	3 (1%) 78 74	44, 60, 104, 133	0
12	Z	222/222 (100%)	-0.38	3 (1%) 78 74	44, 62, 106, 140	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	M	233/246 (94%)	-0.61	1 (0%) 93 91	37, 54, 79, 96	0
13	a	233/246 (94%)	-0.58	1 (0%) 93 91	39, 56, 80, 99	0
14	N	196/196 (100%)	-0.61	2 (1%) 84 81	38, 50, 79, 107	0
14	b	196/196 (100%)	-0.62	3 (1%) 76 71	38, 50, 80, 108	0
All	All	6342/6612 (95%)	-0.39	147 (2%) 64 57	29, 59, 103, 197	0

All (147) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
10	X	1	MET	6.9
10	J	1	MET	6.8
2	B	221	ASP	6.2
1	O	1	MET	5.6
5	E	202	ASP	5.5
3	Q	206	LYS	5.5
12	Z	174	TYR	5.5
9	W	1	SER	5.4
3	C	238	LYS	5.4
2	P	219	ALA	5.4
2	P	51	VAL	5.3
3	Q	50	LEU	5.1
12	L	174	TYR	5.1
3	C	206	LYS	5.0
2	B	218	GLY	4.8
8	V	226	GLU	4.8
3	Q	49	THR	4.8
8	V	222	ASP	4.6
3	C	202	GLN	4.5
9	I	1	SER	4.4
3	C	50	LEU	4.2
2	P	221	ASP	4.2
3	C	49	THR	4.2
3	Q	240	GLU	4.1
3	Q	238	LYS	4.0
10	X	194	ASP	4.0
1	A	1	MET	4.0
3	C	205	ALA	4.0
4	R	117	GLU	4.0
2	B	51	VAL	3.9
1	O	249	ALA	3.8
2	P	220	ASN	3.8

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Mol	Chain	Res	Type	RSRZ
3	C	236	GLN	3.7
8	H	226	GLU	3.7
6	F	181	GLU	3.7
10	X	195	PHE	3.7
2	B	217	LYS	3.6
2	B	219	ALA	3.5
3	Q	48	SER	3.5
3	Q	202	GLN	3.5
3	Q	239	GLN	3.4
3	Q	205	ALA	3.3
13	a	1	THR	3.3
3	Q	225	GLU	3.2
3	Q	141	ASP	3.2
5	S	202	ASP	3.1
8	V	221	CYS	3.1
1	O	2	THR	3.0
3	Q	237	GLU	3.0
2	P	218	GLY	3.0
6	T	181	GLU	3.0
3	C	239	GLN	3.0
2	P	59	ASP	3.0
6	F	202	ASP	3.0
4	R	217	GLN	3.0
4	R	125	LEU	3.0
1	A	249	ALA	3.0
14	b	195	GLN	2.9
10	J	194	ASP	2.9
8	V	224	GLN	2.9
5	S	3	ASN	2.9
12	Z	173	LYS	2.9
2	B	220	ASN	2.9
7	U	242	GLN	2.9
6	T	2	THR	2.8
7	U	2	GLY	2.8
4	R	230	GLU	2.8
6	T	243	ILE	2.8
6	T	201	GLU	2.7
8	H	221	CYS	2.7
4	D	117	GLU	2.7
7	U	222	ASP	2.7
4	R	241	ALA	2.7
2	B	59	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
7	G	3	TYR	2.7
5	S	180	LYS	2.6
13	M	47	ASP	2.6
7	U	203	ASP	2.6
1	A	2	THR	2.6
14	N	105	LYS	2.6
6	T	244	ASN	2.6
4	R	1	ASP	2.6
12	L	173	LYS	2.5
14	N	195	GLN	2.5
7	G	2	GLY	2.5
14	b	105	LYS	2.5
3	Q	236	GLN	2.5
12	L	165	ASN	2.5
3	C	234	ILE	2.5
7	G	222	ASP	2.5
3	C	180	LYS	2.5
5	E	233	ILE	2.5
5	E	122	TYR	2.5
8	V	145	ASP	2.5
9	W	133	LYS	2.5
6	F	205	GLU	2.4
7	G	241	GLU	2.4
6	F	244	ASN	2.4
5	S	173	ARG	2.4
3	C	235	GLU	2.4
5	S	203	GLU	2.4
4	R	54	ASP	2.4
11	K	211	GLY	2.4
2	P	52	THR	2.3
1	A	229	THR	2.3
3	C	225	GLU	2.3
3	C	216	ASP	2.3
2	P	203	SER	2.3
11	Y	146	ASP	2.3
3	C	48	SER	2.3
5	E	180	LYS	2.3
11	Y	182	ASP	2.3
1	O	201	GLU	2.2
4	R	242	GLU	2.2
1	O	231	LYS	2.2
6	T	230	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
3	Q	229	GLN	2.2
4	R	116	GLY	2.2
3	Q	187	GLU	2.2
1	A	231	LYS	2.2
3	Q	181	GLU	2.2
1	A	250	LEU	2.2
4	R	113	LEU	2.2
6	F	201	GLU	2.2
8	H	224	GLN	2.2
8	H	222	ASP	2.1
11	K	107	LYS	2.1
12	Z	167	LYS	2.1
1	A	201	GLU	2.1
10	J	195	PHE	2.1
11	K	30	ARG	2.1
6	F	215	CYS	2.1
14	b	104	ASP	2.1
7	G	179	LYS	2.1
1	O	52	SER	2.1
1	O	178	ARG	2.1
11	Y	201	GLU	2.1
1	O	250	LEU	2.0
8	H	219	ASN	2.0
6	T	241	LYS	2.0
10	J	95	ARG	2.0
9	I	133	LYS	2.0
11	Y	71	GLY	2.0
4	R	2	ARG	2.0
5	E	201	ARG	2.0
10	X	96	ARG	2.0
5	E	163	ARG	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
15	MG	Y	301	1/1	0.84	0.27	6.04	80,80,80,80	0
15	MG	J	201	1/1	0.95	0.21	5.10	56,56,56,56	0
18	MES	Y	303	12/12	0.83	0.27	3.41	58,61,66,67	12
18	MES	K	303	12/12	0.91	0.21	3.04	61,63,68,70	12
17	39V	K	301	46/46	0.91	0.22	2.37	54,66,78,83	0
17	39V	Y	302	46/46	0.90	0.22	1.95	57,67,82,84	0
15	MG	I	301	1/1	0.96	0.18	1.71	63,63,63,63	0
15	MG	N	201	1/1	0.92	0.14	0.50	55,55,55,55	0
15	MG	Z	301	1/1	0.92	0.14	-0.27	64,64,64,64	0
15	MG	K	302	1/1	0.95	0.09	-0.52	56,56,56,56	0
15	MG	G	301	1/1	0.96	0.05	-1.58	60,60,60,60	0
15	MG	L	301	1/1	0.98	0.07	-2.24	63,63,63,63	0
15	MG	I	302	1/1	0.99	0.03	-2.98	59,59,59,59	0
16	CL	G	302	1/1	0.99	0.11	-	43,43,43,43	0
16	CL	U	301	1/1	0.99	0.10	-	44,44,44,44	0

## 6.5 Other polymers

There are no such residues in this entry.