



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 29, 2020 – 07:52 am BST

PDB ID : 5LAJ  
Title : Ligand-induced Lys33-Thr1 crosslinking at the yeast proteasomal subunit beta5 by sulfonate esters  
Authors : Groll, M.; Dubiella, C.; Cui, H.  
Deposited on : 2016-06-14  
Resolution : 2.90 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](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.

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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
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

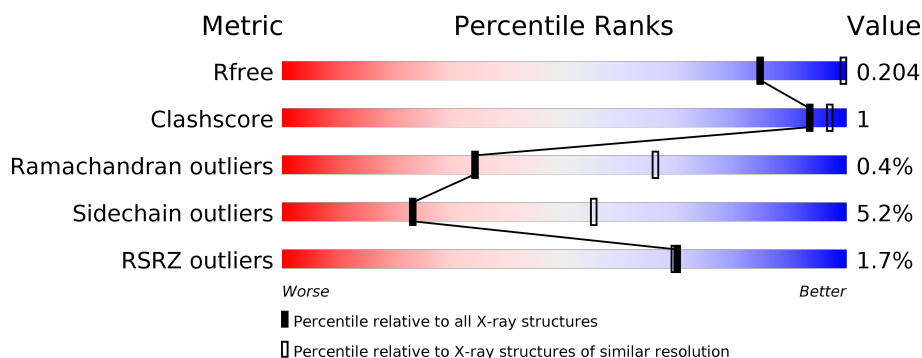
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 Å.

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



















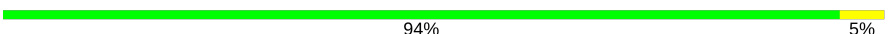
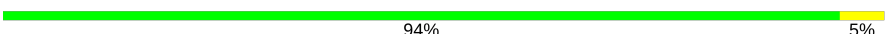



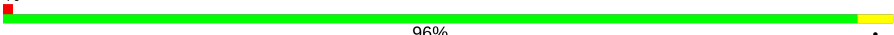
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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 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	<div> <div>2%</div> <div> <div></div> <div>97%</div> <div></div> </div> <div></div> </div>
1	O	250	<div> <div>3%</div> <div> <div></div> <div>97%</div> <div></div> </div> <div></div> </div>
2	B	258	<div> <div>3%</div> <div> <div></div> <div>85%</div> <div>9%</div> <div>5%</div> </div> <div></div> </div>
2	P	258	<div> <div>4%</div> <div> <div></div> <div>87%</div> <div>7%</div> <div>5%</div> </div> <div></div> </div>
3	C	254	<div> <div>4%</div> <div> <div></div> <div>84%</div> <div>9%</div> <div>6%</div> </div> <div></div> </div>
3	Q	254	<div> <div>5%</div> <div> <div></div> <div>83%</div> <div>10%</div> <div>6%</div> </div> <div></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	212	
11	Y	212	
12	L	222	
12	Z	222	
13	M	246	
13	a	246	
14	N	196	
14	b	196	

## 2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 49524 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-5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	212	Total	C	N	O	S	0	0	0
			1643	1045	280	311	7			
11	Y	212	Total	C	N	O	S	0	0	0
			1643	1045	280	311	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	228	Total	C	N	O	S	0	0	0
			1786	1131	305	343	7			
13	a	231	Total	C	N	O	S	0	0	0
			1806	1142	309	348	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	0	0
			1	1		
15	J	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	K	2	Total 2	Mg 2	0	0
15	I	3	Total 3	Mg 3	0	0
15	Z	1	Total 1	Mg 1	0	0
15	N	2	Total 2	Mg 2	0	0
15	L	1	Total 1	Mg 1	0	0

- Molecule 16 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	A	8	Total 8	O 8	0	0
16	B	7	Total 7	O 7	0	0
16	C	7	Total 7	O 7	0	0
16	D	7	Total 7	O 7	0	0
16	E	6	Total 6	O 6	0	0
16	F	6	Total 6	O 6	0	0
16	G	7	Total 7	O 7	0	0
16	H	14	Total 14	O 14	0	0
16	I	5	Total 5	O 5	0	0
16	J	10	Total 10	O 10	0	0
16	K	9	Total 9	O 9	0	0
16	L	11	Total 11	O 11	0	0
16	M	8	Total 8	O 8	0	0
16	N	6	Total 6	O 6	0	0

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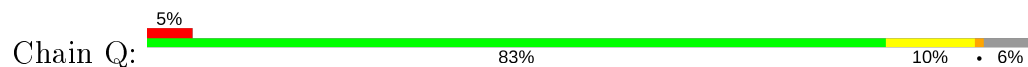
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	O	2	Total 2	O 2	0	0
16	P	9	Total 9	O 9	0	0
16	Q	5	Total 5	O 5	0	0
16	R	3	Total 3	O 3	0	0
16	S	4	Total 4	O 4	0	0
16	T	3	Total 3	O 3	0	0
16	U	10	Total 10	O 10	0	0
16	V	9	Total 9	O 9	0	0
16	W	6	Total 6	O 6	0	0
16	X	5	Total 5	O 5	0	0
16	Y	9	Total 9	O 9	0	0
16	Z	10	Total 10	O 10	0	0
16	a	14	Total 14	O 14	0	0
16	b	5	Total 5	O 5	0	0





GLU  
GLN  
ASP  
LYS  
LYS  
LYS  
LYS  
SER  
ASN  
HIS

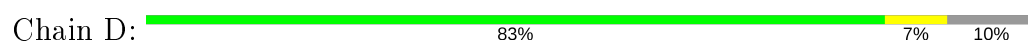
• Molecule 3: Proteasome subunit alpha type-4



MET SER G1 R4 R38 T49 L50 K51 L52 Q53 D84 T55 K61 N77 V124 Q147 T148 E149 P150 Q160 T161 V169 R170 E171 K175 K180 P183 V201 Q202 T203 Q204 A205 K206 V213 E225 T232 Q236 E237 K238 Q239 E240 GLN

GLU  
GLN  
ASP  
LYS  
LYS  
LYS  
SER  
ASN  
HIS

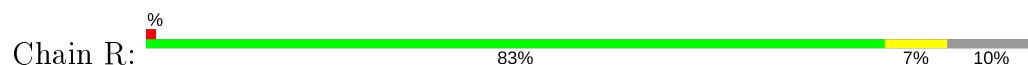
• Molecule 4: Proteasome subunit alpha type-5



MET PHE LEU THR ARG SER GLU TTR D1 L20 L40 L51 C68 A77 I81 H91 I99 L104 E117 GLY ALA SER GLY GLU ARG L125 N160 L176 W179 L190 L193 I214 L235 K236 E242 SER PRQ GLU GLU ALA ASP

VAL  
GLU  
MET  
SER

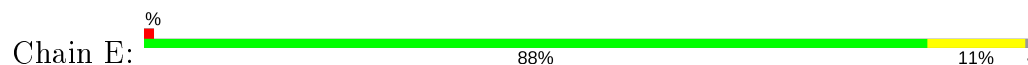
• Molecule 4: Proteasome subunit alpha type-5



MET PHE LEU THR ARG SER GLU TTR D1 L20 L40 L51 C68 A77 I81 I99 L104 E117 GLY ALA SER GLY GLU ARG L125 N160 L176 W179 L190 L193 I214 L235 K236 E242 SER PRQ GLU GLU ALA ASP VAL GLU

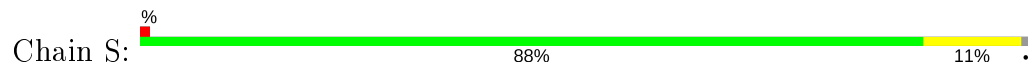
MET  
SER

• Molecule 5: Proteasome subunit alpha type-6



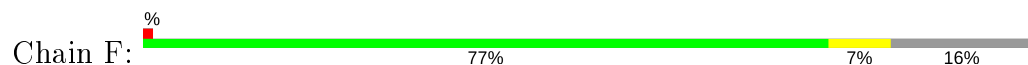
MET PHE ARG N3 D8 T9 V10 F12 L25 K29 E54 L55 L71 L87 N99 A107 Q116 T119 Y122 L155 T158 T174 L175 D176 K180 N184 L188 R201 D202 V207 D208 K217 I233

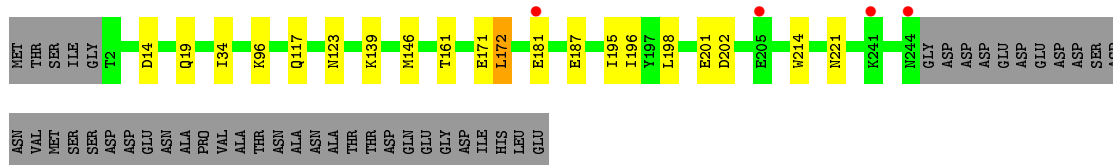
• Molecule 5: Proteasome subunit alpha type-6



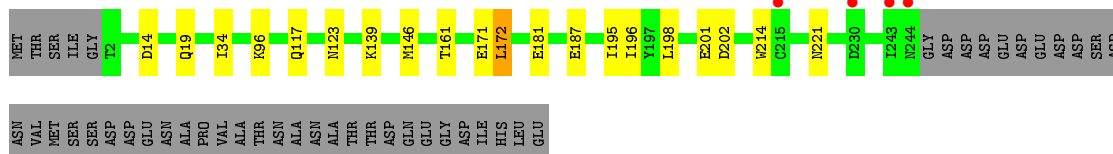
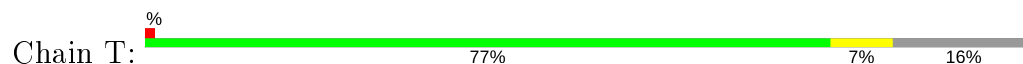
MET PHE ARG N3 D8 T9 V10 F12 L25 K29 E54 L55 L71 L87 N99 A107 Q116 T119 Y122 L155 T158 L175 D176 T177 F178 I179 K180 N184 L188 D202 V207 D208 K217 I233

• Molecule 6: Probable proteasome subunit alpha type-7





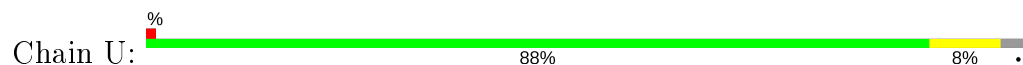
- Molecule 6: Probable proteasome subunit alpha type-7



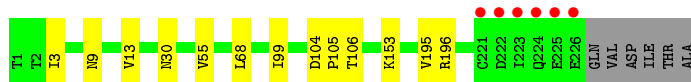
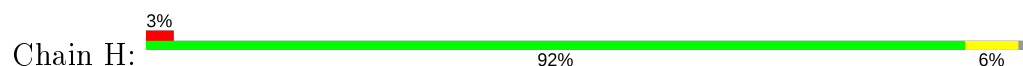
- Molecule 7: Proteasome subunit alpha type-1



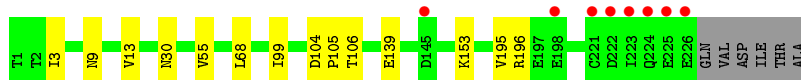
- Molecule 7: Proteasome subunit alpha type-1



- Molecule 8: Proteasome subunit beta type-2



- Molecule 8: Proteasome subunit beta type-2



- Molecule 9: Proteasome subunit beta type-3





- Molecule 9: Proteasome subunit beta type-3

Chain W: 93% 6%



- Molecule 10: Proteasome subunit beta type-4

Chain J: 89% 9% ..



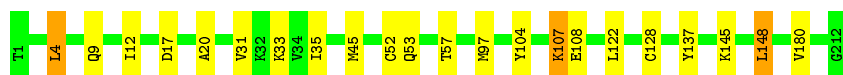
- Molecule 10: Proteasome subunit beta type-4

Chain X: 88% 10% ..



- Molecule 11: Proteasome subunit beta type-5

Chain K: 90% 9% .



- Molecule 11: Proteasome subunit beta type-5

Chain Y: 91% 8% .



- Molecule 12: Proteasome subunit beta type-6

Chain L: 94% 5%




- Molecule 12: Proteasome subunit beta type-6

Chain Z:  94% 5%




- Molecule 13: Proteasome subunit beta type-7

Chain M:  86% 6% 7%

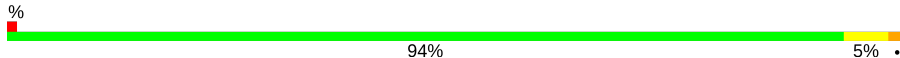


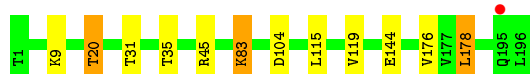
- Molecule 13: Proteasome subunit beta type-7

Chain a:  89% 6% 2%



- Molecule 14: Proteasome subunit beta type-1

Chain N:  94% 5% 1%



- Molecule 14: Proteasome subunit beta type-1

Chain b:  96% 1% 1%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	137.25Å 300.53Å 146.42Å 90.00° 113.73° 90.00°	Depositor
Resolution (Å)	15.00 – 2.90 15.00 – 2.90	Depositor EDS
% Data completeness (in resolution range)	96.8 (15.00-2.90) 96.8 (15.00-2.90)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.69 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, $R_{free}$	0.180 , 0.201 0.185 , 0.204	Depositor DCC
$R_{free}$ test set	11489 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	64.6	Xtriage
Anisotropy	0.056	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 50.7	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	49524	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.40% 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

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	0.48	0/2642
1	O	0.27	0/1952	0.48	0/2642
2	B	0.28	0/1934	0.51	0/2618
2	P	0.27	0/1934	0.52	0/2618
3	C	0.28	0/1910	0.53	0/2586
3	Q	0.28	0/1910	0.53	0/2586
4	D	0.27	0/1837	0.50	0/2475
4	R	0.27	0/1837	0.50	0/2475
5	E	0.27	0/1800	0.50	0/2433
5	S	0.27	0/1800	0.50	0/2433
6	F	0.28	0/1932	0.47	0/2609
6	T	0.28	0/1932	0.47	0/2609
7	G	0.28	0/1945	0.49	0/2634
7	U	0.28	0/1945	0.49	0/2634
8	H	0.26	0/1750	0.50	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	0.50	0/2142
10	X	0.27	0/1589	0.50	0/2142
11	K	0.26	0/1680	0.51	1/2272 (0.0%)
11	Y	0.26	0/1680	0.51	1/2272 (0.0%)
12	L	0.27	0/1795	0.49	0/2420
12	Z	0.27	0/1795	0.49	0/2420
13	M	0.27	0/1817	0.54	0/2465
13	a	0.27	0/1837	0.54	0/2492
14	N	0.26	0/1541	0.48	0/2087
14	b	0.26	0/1541	0.48	0/2087
All	All	0.27	0/50206	0.50	2/67887 (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
2	B	0	1
2	P	0	1
All	All	0	2

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	Y	4	LEU	CA-CB-CG	5.20	127.27	115.30
11	K	4	LEU	CA-CB-CG	5.15	127.16	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	50	LYS	Peptide
2	P	50	LYS	Peptide

## 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	1	0
1	O	1915	0	1929	2	0
2	B	1904	0	1904	10	0
2	P	1904	0	1904	5	0
3	C	1881	0	1895	7	0
3	Q	1881	0	1895	7	0
4	D	1813	0	1797	4	0
4	R	1813	0	1797	3	0
5	E	1773	0	1775	6	0
5	S	1773	0	1775	6	0
6	F	1892	0	1883	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	T	1892	0	1883	4	0
7	G	1907	0	1901	3	0
7	U	1907	0	1901	5	0
8	H	1719	0	1719	2	0
8	V	1719	0	1719	3	0
9	I	1581	0	1574	7	0
9	W	1581	0	1574	6	0
10	J	1561	0	1569	7	0
10	X	1561	0	1569	8	0
11	K	1643	0	1591	9	0
11	Y	1643	0	1591	8	0
12	L	1757	0	1711	2	0
12	Z	1757	0	1711	2	0
13	M	1786	0	1790	5	0
13	a	1806	0	1808	0	0
14	N	1512	0	1481	6	0
14	b	1512	0	1481	0	0
15	G	1	0	0	0	0
15	I	3	0	0	0	0
15	J	1	0	0	0	0
15	K	2	0	0	0	0
15	L	1	0	0	0	0
15	N	2	0	0	0	0
15	Z	1	0	0	0	0
16	A	8	0	0	0	0
16	B	7	0	0	0	0
16	C	7	0	0	0	0
16	D	7	0	0	0	0
16	E	6	0	0	0	0
16	F	6	0	0	0	0
16	G	7	0	0	0	0
16	H	14	0	0	0	0
16	I	5	0	0	0	0
16	J	10	0	0	0	0
16	K	9	0	0	0	0
16	L	11	0	0	0	0
16	M	8	0	0	0	0
16	N	6	0	0	0	0
16	O	2	0	0	0	0
16	P	9	0	0	0	0
16	Q	5	0	0	0	0
16	R	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	S	4	0	0	0	0
16	T	3	0	0	0	0
16	U	10	0	0	0	0
16	V	9	0	0	0	0
16	W	6	0	0	0	0
16	X	5	0	0	0	0
16	Y	9	0	0	0	0
16	Z	10	0	0	0	0
16	a	14	0	0	0	0
16	b	5	0	0	0	0
All	All	49524	0	49056	119	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.

The worst 5 of 119 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:51:LYS:O	3:C:52:LEU:HB2	1.99	0.61
10:X:126:VAL:HG12	10:X:128:LEU:HG	1.82	0.61
10:J:126:VAL:HG12	10:J:128:LEU:HG	1.82	0.61
3:Q:51:LYS:O	3:Q:52:LEU:HB2	1.99	0.61
2:B:12:PHE:H	3:C:17:GLN:HE22	1.49	0.61

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%)	240 (97%)	6 (2%)	2 (1%)	19 51
1	O	248/250 (99%)	240 (97%)	6 (2%)	2 (1%)	19 51

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	242/258 (94%)	234 (97%)	4 (2%)	4 (2%)	9	31
2	P	242/258 (94%)	233 (96%)	5 (2%)	4 (2%)	9	31
3	C	238/254 (94%)	231 (97%)	4 (2%)	3 (1%)	12	37
3	Q	238/254 (94%)	231 (97%)	4 (2%)	3 (1%)	12	37
4	D	231/260 (89%)	227 (98%)	4 (2%)	0	100	100
4	R	231/260 (89%)	227 (98%)	4 (2%)	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%)	236 (98%)	5 (2%)	0	100	100
6	T	241/288 (84%)	237 (98%)	4 (2%)	0	100	100
7	G	239/252 (95%)	236 (99%)	3 (1%)	0	100	100
7	U	239/252 (95%)	237 (99%)	2 (1%)	0	100	100
8	H	224/232 (97%)	217 (97%)	6 (3%)	1 (0%)	34	66
8	V	224/232 (97%)	217 (97%)	6 (3%)	1 (0%)	34	66
9	I	202/205 (98%)	196 (97%)	6 (3%)	0	100	100
9	W	202/205 (98%)	196 (97%)	6 (3%)	0	100	100
10	J	193/198 (98%)	188 (97%)	5 (3%)	0	100	100
10	X	193/198 (98%)	188 (97%)	5 (3%)	0	100	100
11	K	210/212 (99%)	203 (97%)	7 (3%)	0	100	100
11	Y	210/212 (99%)	203 (97%)	7 (3%)	0	100	100
12	L	220/222 (99%)	216 (98%)	3 (1%)	1 (0%)	29	61
12	Z	220/222 (99%)	216 (98%)	3 (1%)	1 (0%)	29	61
13	M	226/246 (92%)	219 (97%)	7 (3%)	0	100	100
13	a	229/246 (93%)	222 (97%)	5 (2%)	2 (1%)	17	48
14	N	194/196 (99%)	190 (98%)	4 (2%)	0	100	100
14	b	194/196 (99%)	190 (98%)	4 (2%)	0	100	100
All	All	6277/6614 (95%)	6118 (98%)	135 (2%)	24 (0%)	34	66

5 of 24 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	THR
2	B	218	GLY

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Mol	Chain	Res	Type
2	B	222	GLY
3	C	202	GLN
1	O	2	THR

### 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%)	205 (98%)	4 (2%)	57	84
1	O	209/209 (100%)	205 (98%)	4 (2%)	57	84
2	B	203/216 (94%)	193 (95%)	10 (5%)	25	57
2	P	203/216 (94%)	193 (95%)	10 (5%)	25	57
3	C	212/226 (94%)	195 (92%)	17 (8%)	12	33
3	Q	212/226 (94%)	195 (92%)	17 (8%)	12	33
4	D	194/215 (90%)	180 (93%)	14 (7%)	14	39
4	R	194/215 (90%)	180 (93%)	14 (7%)	14	39
5	E	190/193 (98%)	173 (91%)	17 (9%)	9	29
5	S	190/193 (98%)	174 (92%)	16 (8%)	11	31
6	F	201/239 (84%)	187 (93%)	14 (7%)	15	41
6	T	201/239 (84%)	187 (93%)	14 (7%)	15	41
7	G	206/210 (98%)	195 (95%)	11 (5%)	22	54
7	U	206/210 (98%)	195 (95%)	11 (5%)	22	54
8	H	185/190 (97%)	177 (96%)	8 (4%)	29	62
8	V	185/190 (97%)	177 (96%)	8 (4%)	29	62
9	I	172/173 (99%)	168 (98%)	4 (2%)	50	80
9	W	172/173 (99%)	168 (98%)	4 (2%)	50	80
10	J	173/175 (99%)	166 (96%)	7 (4%)	31	65
10	X	173/175 (99%)	166 (96%)	7 (4%)	31	65
11	K	168/169 (99%)	161 (96%)	7 (4%)	30	63

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	Y	168/169 (99%)	161 (96%)	7 (4%)	30	63
12	L	185/185 (100%)	176 (95%)	9 (5%)	25	57
12	Z	185/185 (100%)	176 (95%)	9 (5%)	25	57
13	M	195/208 (94%)	186 (95%)	9 (5%)	27	60
13	a	197/208 (95%)	188 (95%)	9 (5%)	27	60
14	N	162/162 (100%)	155 (96%)	7 (4%)	29	62
14	b	162/162 (100%)	155 (96%)	7 (4%)	29	62
All	All	5312/5540 (96%)	5037 (95%)	275 (5%)	23	55

5 of 275 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
13	M	48	ASN
3	Q	38	ASN
12	Z	108	HIS
13	M	187	ARG
1	O	61	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 97 such sidechains are listed below:

Mol	Chain	Res	Type
12	L	3	ASN
3	Q	17	GLN
11	Y	208	ASN
13	M	48	ASN
2	P	58	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 [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 11 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 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%)	-0.39	5 (2%) 65 63	38, 54, 92, 131	0
1	O	250/250 (100%)	-0.36	7 (2%) 53 49	46, 64, 109, 144	0
2	B	244/258 (94%)	-0.35	8 (3%) 46 41	40, 61, 109, 177	0
2	P	244/258 (94%)	-0.22	10 (4%) 37 32	47, 65, 115, 178	0
3	C	240/254 (94%)	-0.18	11 (4%) 32 29	41, 66, 134, 164	0
3	Q	240/254 (94%)	-0.04	13 (5%) 25 22	46, 76, 156, 178	0
4	D	235/260 (90%)	-0.37	1 (0%) 92 93	48, 68, 104, 145	0
4	R	235/260 (90%)	-0.27	2 (0%) 84 84	51, 72, 112, 144	0
5	E	231/234 (98%)	-0.29	3 (1%) 77 77	52, 72, 109, 149	0
5	S	231/234 (98%)	-0.21	3 (1%) 77 77	53, 78, 122, 168	0
6	F	243/288 (84%)	-0.45	4 (1%) 72 71	42, 60, 107, 146	0
6	T	243/288 (84%)	-0.34	4 (1%) 72 71	44, 69, 128, 164	0
7	G	241/252 (95%)	-0.50	1 (0%) 92 93	41, 56, 93, 134	0
7	U	241/252 (95%)	-0.44	3 (1%) 79 79	43, 59, 97, 130	0
8	H	226/232 (97%)	-0.34	6 (2%) 54 50	43, 55, 94, 170	0
8	V	226/232 (97%)	-0.22	8 (3%) 44 38	45, 60, 99, 185	0
9	I	204/205 (99%)	-0.65	1 (0%) 91 91	38, 52, 82, 111	0
9	W	204/205 (99%)	-0.60	1 (0%) 91 91	40, 56, 91, 114	0
10	J	195/198 (98%)	-0.48	2 (1%) 82 82	39, 58, 86, 144	0
10	X	195/198 (98%)	-0.42	3 (1%) 73 73	39, 61, 90, 150	0
11	K	212/212 (100%)	-0.47	0 100 100	42, 58, 83, 100	0
11	Y	212/212 (100%)	-0.51	0 100 100	41, 56, 81, 104	0
12	L	222/222 (100%)	-0.53	1 (0%) 91 91	42, 58, 92, 141	0
12	Z	222/222 (100%)	-0.47	1 (0%) 91 91	34, 57, 90, 129	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	M	228/246 (92%)	-0.52	2 (0%) 84 84	37, 56, 85, 102	0
13	a	231/246 (93%)	-0.50	4 (1%) 70 69	38, 57, 86, 109	0
14	N	196/196 (100%)	-0.55	1 (0%) 91 91	38, 52, 85, 121	0
14	b	196/196 (100%)	-0.49	1 (0%) 91 91	40, 53, 85, 119	0
All	All	6337/6614 (95%)	-0.39	106 (1%) 70 69	34, 61, 106, 185	0

The worst 5 of 106 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
8	V	224	GLN	9.0
10	X	1	MET	8.7
3	Q	206	LYS	7.6
8	V	226	GLU	7.5
3	Q	49	THR	7.5

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
15	MG	I	302	1/1	0.71	0.22	110,110,110,110	0
15	MG	N	202	1/1	0.81	0.38	69,69,69,69	0
15	MG	K	302	1/1	0.86	0.48	70,70,70,70	0
15	MG	N	201	1/1	0.94	0.12	50,50,50,50	0
15	MG	Z	301	1/1	0.96	0.28	64,64,64,64	0
15	MG	G	301	1/1	0.97	0.07	55,55,55,55	0
15	MG	J	201	1/1	0.97	0.21	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
15	MG	L	301	1/1	0.97	0.07	67,67,67,67	0
15	MG	I	301	1/1	0.99	0.46	71,71,71,71	0
15	MG	K	301	1/1	0.99	0.10	57,57,57,57	0
15	MG	I	303	1/1	0.99	0.06	46,46,46,46	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.