



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 13, 2020 – 04:08 pm BST

PDB ID : 4Y69  
Title : Yeast 20S proteasome in complex with Ac-PAD-ep  
Authors : Huber, E.M.; Groll, M.  
Deposited on : 2015-02-12  
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.

---

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
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

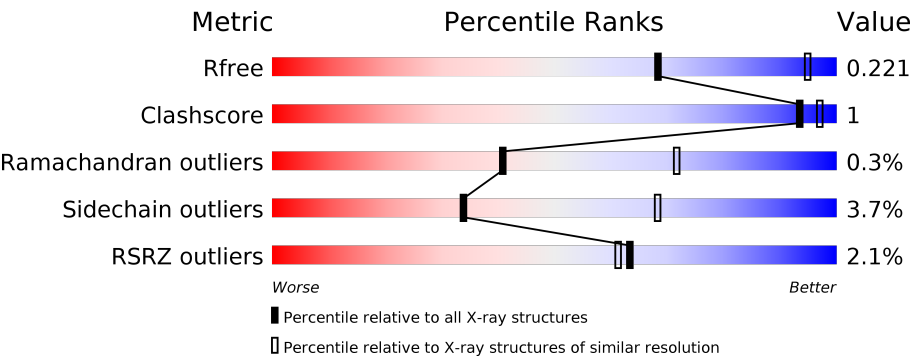
# 1 Overall quality at a glance i

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>4%</div><div><div></div><div>98%</div><div></div><div></div></div><div></div></div>
1	O	250	<div><div>2%</div><div><div></div><div>98%</div><div></div><div></div></div><div></div></div>
2	B	258	<div><div>4%</div><div><div></div><div>86%</div><div>9%</div><div>5%</div></div><div></div></div>
2	P	258	<div><div>3%</div><div><div></div><div>87%</div><div>7%</div><div>5%</div></div><div></div></div>
3	C	254	<div><div>5%</div><div><div></div><div>86%</div><div>7%</div><div>6%</div></div><div></div></div>
3	Q	254	<div><div>6%</div><div><div></div><div>87%</div><div>7%</div><div>6%</div></div><div></div></div>

Continued on next page...

Continued from previous page...

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	
15	c	4	
15	d	4	

## 2 Entry composition

There are 18 unique types of molecules in this entry. The entry contains 49849 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	1	0
			1726	1087	300	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			

*Continued on next page...*

*Continued from previous page...*

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	233	Total	C	N	O	S	0	0	0
			1824	1154	312	351	7			
13	a	233	Total	C	N	O	S	0	0	0
			1824	1154	312	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 a protein called Ac-PAD-ep.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	c	4	Total	C	N	O	0	0	0
			27	17	3	7			
15	d	4	Total	C	N	O	0	0	0
			27	17	3	7			

- Molecule 16 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 17 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 18 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
18	A	13	Total 13	O 13	0	0
18	B	9	Total 9	O 9	0	0
18	C	20	Total 20	O 20	0	0
18	D	9	Total 9	O 9	0	0
18	E	6	Total 6	O 6	0	0
18	F	15	Total 15	O 15	0	0
18	G	24	Total 24	O 24	0	0
18	H	20	Total 20	O 20	0	0
18	I	16	Total 16	O 16	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
18	J	20	Total 20	O 20	0	0
18	K	9	Total 9	O 9	0	0
18	L	20	Total 20	O 20	0	0
18	M	20	Total 20	O 20	0	0
18	N	18	Total 18	O 18	0	0
18	O	5	Total 5	O 5	0	0
18	P	13	Total 13	O 13	0	0
18	Q	11	Total 11	O 11	0	0
18	R	16	Total 16	O 16	0	0
18	S	6	Total 6	O 6	0	0
18	T	15	Total 15	O 15	0	0
18	U	19	Total 19	O 19	0	0
18	V	14	Total 14	O 14	0	0
18	W	9	Total 9	O 9	0	0
18	X	18	Total 18	O 18	0	0
18	Y	22	Total 22	O 22	0	0
18	Z	14	Total 14	O 14	0	0
18	a	18	Total 18	O 18	0	0
18	b	11	Total 11	O 11	0	0
18	c	2	Total 2	O 2	0	0
18	d	1	Total 1	O 1	0	0





GLU  
GLN  
ASP  
LYS  
LYS  
LYS  
SER  
ASN  
HIS

• Molecule 3: Proteasome subunit alpha type-4

Chain Q: 6% 87% 7% 6%

MET SER G1 R4 K35 N38 R47 S48 T49 L50 K51 L52 T55 N77 V124 Q147 T148 E149 P150 S158 A159 Q160 V169 K180 E187 V201 Q202 T203 G204 A205 K206 E225 Q229 Q235 E237 K238 Q239 E240 GLN GLN GLN ASP LYS

LYS  
LYS  
LYS  
SER  
ASN  
HIS

• Molecule 4: Proteasome subunit alpha type-5

Chain D: 2% 85% 10%

MET PHE LEU ARG SER GLU TTR D1 T47 L51 H91 I99 E117 E117 GLY ALA SER GLY GLY GLU ARG L125 D143 Y159 N160 L176 W179 L193 I214 D224 L235 K236 A241 E242 SER PRO GLU GLU ALA ASP VAL MET SER

• Molecule 4: Proteasome subunit alpha type-5

Chain R: 2% 85% 5% 10%

MET PHE LEU ARG SER GLU TTR D1 L51 H91 T99 E117 GLY ALA SER GLY GLU GLU ARG L125 D143 Y159 N160 L176 W179 L193 I214 Q217 L235 K236 A241 E242 SER PRO GLU GLU ALA ASP VAL MET SER

• Molecule 5: Proteasome subunit alpha type-6

Chain E: 3% 91% 8%

MET PHE ARG N3 T9 F12 K29 L55 L71 A77 P78 L87 N99 A107 Y122 G123 L175 F178 N184 L188 R201 D202 V207 D208 E227 K231 Y232 I233

• Molecule 5: Proteasome subunit alpha type-6

Chain S: 4% 91% 8%

MET PHE ARG N3 T9 F12 K29 H51 L55 S56 S57 Y58 L71 A77 P78 L87 N99 A107 R173 T174 L175 F178 N184 L188 E194 D202 E203 S204 V207 D208 D218 E227 K231 Y232 I233

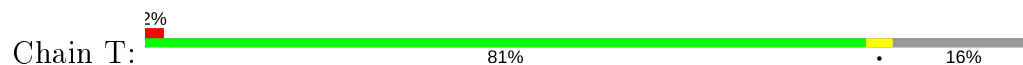
• Molecule 6: Probable proteasome subunit alpha type-7

Chain F: 2% 81% 16%

MET THR SER ILE T2 Q19 Q117 N123 K139 L172 D177 E181 E201 D202 E205 K206 D207 K214 Q240 K244 GLY ASP ASP ASP GLU ASP GLU ASP ASP SER ASP ASN VAL MET SER SER ASP ASP ASP GLU ASN ASP VAL ALA THR ALA

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

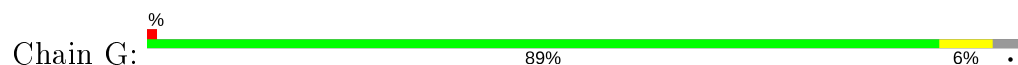
- Molecule 6: Probable proteasome subunit alpha type-7



MET THR ASN THR ILE GLY T2 Q19 Q117 Q117 N123 K139 L172 H178 E181 E201 D202 D207 W214 C215 D230 Q240 R241 E242 I243 N244 GLY ASP ASP ASP GLU ASP ASP GLU ASP ASP ASP ASP SER ASP ASP ASN VAL MET SER SER ASP ASP ASN ALA VAL VAL ALA

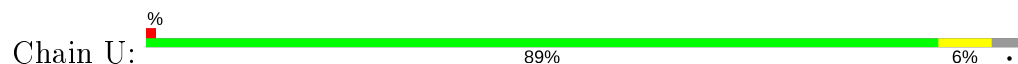
THR ASN ALA ALA THR THR ASP GLN GLU GLY ASP ASP ILE HIS LEU GLU

- Molecule 7: Proteasome subunit alpha type-1



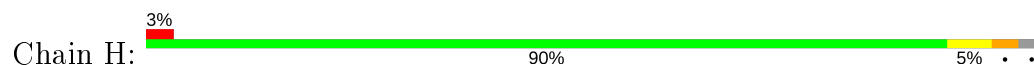
MET SER SER GLY ALA ALA ALA ALA SER ALA ALA ALA G2 Y3 F23 T26 R63 R75 I78 P79 F78 N83 L115 S116 Q117 R122 M125 D149 P150 K179 E208 R235 L236 Q242 ASP

- Molecule 7: Proteasome subunit alpha type-1



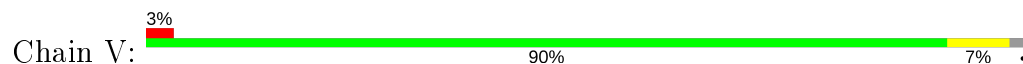
MET SER SER GLY ALA ALA ALA ALA SER ALA ALA ALA G2 P12 F23 T26 R75 I78 P79 N83 L115 S116 Q117 R122 M125 D149 P150 K181 E208 D222 R235 L236 Q242 ASP

- Molecule 8: Proteasome subunit beta type-2



T1 R30 R35 A50 E53 A54 V55 Q57 L68 Y97 D104 P105 H114 A115 H116 G117 S118 T119 D120 R196 R197 E198 C221 D222 I223 Q224 E225 E226 GLN VAL ASP ILE THR ALA

- Molecule 8: Proteasome subunit beta type-2



T1 R30 R35 E53 A54 V55 Q57 L68 R94 D104 P105 S112 I113 T119 D120 E139 D145 R196 V218 C221 D222 I223 Q224 E225 E226 GLN VAL ASP ILE THR ALA

- Molecule 9: Proteasome subunit beta type-3

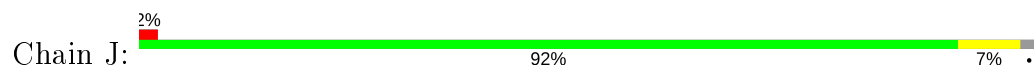


MET S1 G9 I10 V20 S36 N37 K41 R98 P118 I126 E131 A141 E150 L171 D204

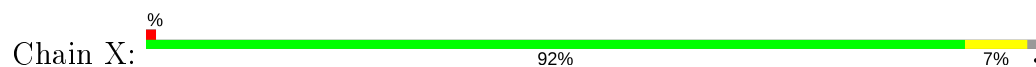
- Molecule 9: Proteasome subunit beta type-3



- Molecule 10: Proteasome subunit beta type-4



- Molecule 10: Proteasome subunit beta type-4



- Molecule 11: Proteasome subunit beta type-5



- Molecule 11: Proteasome subunit beta type-5




- Molecule 12: Proteasome subunit beta type-6

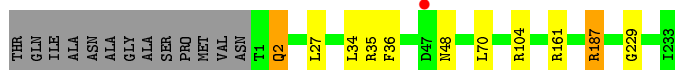


- Molecule 12: Proteasome subunit beta type-6



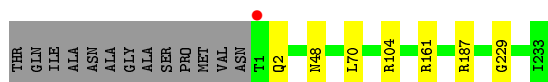
- Molecule 13: Proteasome subunit beta type-7

Chain M:  90% • • 5%



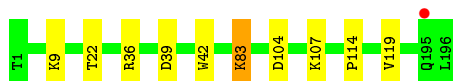
- Molecule 13: Proteasome subunit beta type-7

Chain a:  92% • 5%



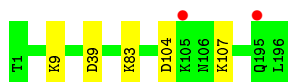
- Molecule 14: Proteasome subunit beta type-1

Chain N:  95% 5% •



- Molecule 14: Proteasome subunit beta type-1

Chain b:  97% •



- Molecule 15: Ac-PAD-ep

Chain c:  100%

There are no outlier residues recorded for this chain.

- Molecule 15: Ac-PAD-ep

Chain d:  100%

There are no outlier residues recorded for this chain.

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	136.68Å 301.26Å 145.94Å 90.00° 113.23° 90.00°	Depositor
Resolution (Å)	15.00 – 2.90 15.00 – 2.90	Depositor EDS
% Data completeness (in resolution range)	94.2 (15.00-2.90) 94.3 (15.00-2.90)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.42 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, $R_{free}$	0.195 , 0.217 0.201 , 0.221	Depositor DCC
$R_{free}$ test set	11173 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	52.6	Xtriage
Anisotropy	0.097	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 36.6	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	0.93	EDS
Total number of atoms	49849	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.49% 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: ASJ, MG, N7P, POL, 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	0.28	0/1952	0.46	0/2642
1	O	0.27	0/1952	0.46	0/2642
2	B	0.28	0/1934	0.50	0/2618
2	P	0.28	0/1934	0.50	0/2618
3	C	0.28	0/1910	0.51	0/2586
3	Q	0.27	0/1910	0.50	0/2586
4	D	0.27	0/1837	0.48	0/2475
4	R	0.27	0/1837	0.48	0/2475
5	E	0.27	0/1800	0.47	0/2433
5	S	0.27	0/1800	0.47	0/2433
6	F	0.27	0/1932	0.45	0/2609
6	T	0.27	0/1932	0.45	0/2609
7	G	0.27	0/1945	0.47	0/2634
7	U	0.28	0/1945	0.47	0/2634
8	H	0.50	2/1761 (0.1%)	0.65	6/2388 (0.3%)
8	V	0.29	0/1750	0.48	0/2373
9	I	0.30	0/1611	0.49	0/2174
9	W	0.29	0/1611	0.49	0/2174
10	J	0.27	0/1589	0.48	0/2142
10	X	0.27	0/1589	0.48	0/2142
11	K	0.27	0/1681	0.51	0/2274
11	Y	0.28	0/1681	0.51	0/2274
12	L	0.30	0/1795	0.49	0/2420
12	Z	0.28	0/1795	0.48	0/2420
13	M	0.28	0/1855	0.51	0/2514
13	a	0.29	0/1855	0.51	0/2514
14	N	0.35	0/1541	0.51	0/2087
14	b	0.29	0/1541	0.49	0/2087
15	c	1.18	0/4	1.01	0/4
15	d	1.46	0/4	2.02	0/4
All	All	0.29	2/50283 (0.0%)	0.49	6/67985 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	H	114[A]	HIS	CA-C	9.90	1.78	1.52
8	H	114[B]	HIS	CA-C	9.90	1.78	1.52

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	H	114[A]	HIS	CA-C-O	10.04	141.18	120.10
8	H	114[B]	HIS	CA-C-O	10.04	141.18	120.10
8	H	114[A]	HIS	CA-C-N	-7.85	99.94	117.20
8	H	114[B]	HIS	CA-C-N	-7.85	99.94	117.20
8	H	114[A]	HIS	CB-CA-C	-5.86	98.68	110.40

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	1	0
1	O	1915	0	1929	2	0
2	B	1904	0	1904	13	0
2	P	1904	0	1904	9	0
3	C	1881	0	1895	10	0
3	Q	1881	0	1895	6	0
4	D	1813	0	1797	4	0
4	R	1813	0	1797	4	0
5	E	1773	0	1775	6	0
5	S	1773	0	1775	5	0
6	F	1892	0	1883	1	0
6	T	1892	0	1883	2	0
7	G	1907	0	1901	4	0
7	U	1907	0	1901	4	0
8	H	1726	0	1726	19	0
8	V	1719	0	1719	11	0
9	I	1581	0	1574	7	0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	W	1581	0	1574	7	0
10	J	1561	0	1569	6	0
10	X	1561	0	1569	6	0
11	K	1644	0	1595	6	0
11	Y	1644	0	1595	6	0
12	L	1757	0	1711	0	0
12	Z	1757	0	1711	0	0
13	M	1824	0	1832	6	0
13	a	1824	0	1832	0	0
14	N	1512	0	1479	5	0
14	b	1512	0	1478	0	0
15	c	27	0	14	0	0
15	d	27	0	14	0	0
16	G	1	0	0	0	0
16	I	2	0	0	0	0
16	K	1	0	0	0	0
16	L	1	0	0	0	0
16	N	1	0	0	0	0
16	Z	1	0	0	0	0
17	G	1	0	0	0	0
17	U	1	0	0	0	0
18	A	13	0	0	0	0
18	B	9	0	0	0	0
18	C	20	0	0	0	0
18	D	9	0	0	0	0
18	E	6	0	0	0	0
18	F	15	0	0	0	0
18	G	24	0	0	0	0
18	H	20	0	0	1	0
18	I	16	0	0	0	0
18	J	20	0	0	0	0
18	K	9	0	0	0	0
18	L	20	0	0	0	0
18	M	20	0	0	1	0
18	N	18	0	0	0	0
18	O	5	0	0	0	0
18	P	13	0	0	1	0
18	Q	11	0	0	0	0
18	R	16	0	0	0	0
18	S	6	0	0	0	0
18	T	15	0	0	1	0
18	U	19	0	0	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	V	14	0	0	0	0
18	W	9	0	0	0	0
18	X	18	0	0	0	0
18	Y	22	0	0	0	0
18	Z	14	0	0	0	0
18	a	18	0	0	0	0
18	b	11	0	0	0	0
18	c	2	0	0	0	0
18	d	1	0	0	0	0
All	All	49849	0	49160	124	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 124 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)
8:H:118:SER:OG	18:H:301:HOH:O	1.87	0.91
8:H:114[A]:HIS:CA	8:H:115:ALA:N	2.38	0.86
8:H:53:GLU:OE1	8:H:57:GLN:NE2	2.24	0.69
8:H:53:GLU:O	8:H:57:GLN:HG3	1.94	0.68
8:V:53:GLU:O	8:V:57:GLN:HG3	1.94	0.68

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%)	238 (96%)	9 (4%)	1 (0%)	34 66
1	O	248/250 (99%)	238 (96%)	9 (4%)	1 (0%)	34 66

*Continued on next page...*

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	242/258 (94%)	233 (96%)	5 (2%)	4 (2%)	9	31
2	P	242/258 (94%)	233 (96%)	5 (2%)	4 (2%)	9	31
3	C	238/254 (94%)	233 (98%)	3 (1%)	2 (1%)	19	51
3	Q	238/254 (94%)	233 (98%)	3 (1%)	2 (1%)	19	51
4	D	231/260 (89%)	227 (98%)	4 (2%)	0	100	100
4	R	231/260 (89%)	228 (99%)	3 (1%)	0	100	100
5	E	229/234 (98%)	223 (97%)	6 (3%)	0	100	100
5	S	229/234 (98%)	223 (97%)	6 (3%)	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%)	239 (100%)	0	0	100	100
7	U	239/252 (95%)	239 (100%)	0	0	100	100
8	H	225/232 (97%)	218 (97%)	6 (3%)	1 (0%)	34	66
8	V	224/232 (97%)	218 (97%)	6 (3%)	0	100	100
9	I	202/205 (98%)	195 (96%)	7 (4%)	0	100	100
9	W	202/205 (98%)	195 (96%)	7 (4%)	0	100	100
10	J	193/198 (98%)	189 (98%)	3 (2%)	1 (0%)	29	61
10	X	193/198 (98%)	189 (98%)	3 (2%)	1 (0%)	29	61
11	K	210/212 (99%)	206 (98%)	4 (2%)	0	100	100
11	Y	210/212 (99%)	206 (98%)	4 (2%)	0	100	100
12	L	220/222 (99%)	215 (98%)	5 (2%)	0	100	100
12	Z	220/222 (99%)	215 (98%)	5 (2%)	0	100	100
13	M	231/246 (94%)	224 (97%)	6 (3%)	1 (0%)	34	66
13	a	231/246 (94%)	224 (97%)	6 (3%)	1 (0%)	34	66
14	N	194/196 (99%)	188 (97%)	6 (3%)	0	100	100
14	b	194/196 (99%)	189 (97%)	5 (3%)	0	100	100
15	c	1/4 (25%)	1 (100%)	0	0	100	100
15	d	1/4 (25%)	1 (100%)	0	0	100	100
All	All	6287/6622 (95%)	6133 (98%)	135 (2%)	19 (0%)	41	71

5 of 19 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	51	VAL
2	B	222	GLY
3	C	202	GLN
2	P	51	VAL
2	P	222	GLY

### 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%)	67	89
1	O	209/209 (100%)	206 (99%)	3 (1%)	67	89
2	B	203/216 (94%)	198 (98%)	5 (2%)	47	78
2	P	203/216 (94%)	198 (98%)	5 (2%)	47	78
3	C	212/226 (94%)	202 (95%)	10 (5%)	26	59
3	Q	212/226 (94%)	201 (95%)	11 (5%)	23	55
4	D	194/215 (90%)	184 (95%)	10 (5%)	23	55
4	R	194/215 (90%)	184 (95%)	10 (5%)	23	55
5	E	190/193 (98%)	179 (94%)	11 (6%)	20	50
5	S	190/193 (98%)	179 (94%)	11 (6%)	20	50
6	F	201/239 (84%)	191 (95%)	10 (5%)	24	57
6	T	201/239 (84%)	191 (95%)	10 (5%)	24	57
7	G	206/210 (98%)	196 (95%)	10 (5%)	25	57
7	U	206/210 (98%)	196 (95%)	10 (5%)	25	57
8	H	186/190 (98%)	179 (96%)	7 (4%)	33	67
8	V	185/190 (97%)	179 (97%)	6 (3%)	39	73
9	I	172/173 (99%)	169 (98%)	3 (2%)	60	86
9	W	172/173 (99%)	169 (98%)	3 (2%)	60	86
10	J	173/175 (99%)	168 (97%)	5 (3%)	42	76
10	X	173/175 (99%)	168 (97%)	5 (3%)	42	76

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	K	169/169 (100%)	161 (95%)	8 (5%)	26	59
11	Y	169/169 (100%)	161 (95%)	8 (5%)	26	59
12	L	185/185 (100%)	179 (97%)	6 (3%)	39	73
12	Z	185/185 (100%)	180 (97%)	5 (3%)	44	77
13	M	199/208 (96%)	193 (97%)	6 (3%)	41	75
13	a	199/208 (96%)	193 (97%)	6 (3%)	41	75
14	N	162/162 (100%)	156 (96%)	6 (4%)	34	68
14	b	162/162 (100%)	157 (97%)	5 (3%)	40	74
All	All	5321/5540 (96%)	5123 (96%)	198 (4%)	34	68

5 of 198 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
13	M	48	ASN
3	Q	50	LEU
12	Z	3	ASN
13	M	161	ARG
1	O	122	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 103 such sidechains are listed below:

Mol	Chain	Res	Type
11	K	208	ASN
2	P	58	GLN
11	Y	208	ASN
12	L	3	ASN
13	M	179	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues are modelled in this entry.

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	$\# Z  > 2$
15	N7P	c	1	15	9,10,11	2.24	2 (22%)	9,13,15	2.11	3 (33%)
15	N7P	d	1	15	9,10,11	2.26	4 (44%)	9,13,15	2.03	2 (22%)
15	ASJ	d	3	15,14	4,7,7	1.85	1 (25%)	3,8,8	1.66	1 (33%)
15	ASJ	c	3	15,14	4,7,7	2.17	1 (25%)	3,8,8	2.85	1 (33%)

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
15	N7P	c	1	15	-	0/4/16/18	0/1/1/1
15	N7P	d	1	15	-	0/4/16/18	0/1/1/1
15	ASJ	d	3	15,14	-	0/4/6/6	-
15	ASJ	c	3	15,14	-	2/4/6/6	-

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	c	1	N7P	CA-N	-5.56	1.43	1.48
15	d	1	N7P	CA-N	-4.23	1.44	1.48
15	c	3	ASJ	C-CA	3.91	1.58	1.52
15	d	3	ASJ	C-CA	3.15	1.57	1.52
15	d	1	N7P	CB-CA	-2.95	1.46	1.53

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	c	3	ASJ	CG-CB-CA	4.92	118.16	112.95
15	c	1	N7P	O1-C1-N	4.70	125.76	120.64
15	d	1	N7P	CB-CA-C	-3.78	107.50	112.70
15	d	1	N7P	O1-C1-N	3.33	124.27	120.64
15	c	1	N7P	C2-C1-N	-2.32	115.44	117.87

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	c	3	ASJ	O-C-CA-CB
15	c	3	ASJ	O-C-CA-N

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 9 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%)	-0.34	9 (3%) 42 37	31, 45, 81, 118	0
1	O	250/250 (100%)	-0.25	4 (1%) 72 71	36, 55, 98, 126	0
2	B	244/258 (94%)	-0.21	11 (4%) 33 29	32, 53, 99, 143	0
2	P	244/258 (94%)	-0.14	9 (3%) 41 37	41, 59, 104, 146	0
3	C	240/254 (94%)	-0.10	12 (5%) 28 25	33, 58, 121, 145	0
3	Q	240/254 (94%)	0.13	16 (6%) 17 13	41, 69, 146, 168	0
4	D	235/260 (90%)	-0.23	5 (2%) 63 61	41, 63, 98, 142	0
4	R	235/260 (90%)	-0.11	4 (1%) 70 69	46, 67, 106, 141	0
5	E	231/234 (98%)	-0.13	6 (2%) 56 52	42, 64, 101, 144	0
5	S	231/234 (98%)	-0.04	10 (4%) 35 31	42, 68, 115, 158	0
6	F	243/288 (84%)	-0.28	6 (2%) 57 55	36, 53, 104, 132	0
6	T	243/288 (84%)	-0.15	7 (2%) 51 47	37, 64, 117, 149	0
7	G	241/252 (95%)	-0.39	2 (0%) 86 86	28, 48, 82, 129	0
7	U	241/252 (95%)	-0.33	3 (1%) 79 79	35, 52, 86, 130	0
8	H	226/232 (97%)	-0.31	7 (3%) 49 44	26, 44, 79, 138	0
8	V	226/232 (97%)	-0.27	7 (3%) 49 44	33, 48, 82, 161	0
9	I	204/205 (99%)	-0.59	1 (0%) 91 91	30, 42, 71, 97	0
9	W	204/205 (99%)	-0.55	2 (0%) 82 82	32, 46, 77, 103	0
10	J	195/198 (98%)	-0.46	3 (1%) 73 73	31, 48, 72, 123	0
10	X	195/198 (98%)	-0.39	2 (1%) 82 82	33, 49, 73, 135	0
11	K	212/212 (100%)	-0.44	0 100 100	29, 48, 71, 93	0
11	Y	212/212 (100%)	-0.51	0 100 100	32, 47, 72, 94	0
12	L	222/222 (100%)	-0.45	1 (0%) 91 91	32, 49, 83, 116	0
12	Z	222/222 (100%)	-0.44	2 (0%) 84 84	30, 47, 76, 110	0

*Continued on next page...*



Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	M	233/246 (94%)	-0.54	1 (0%) 92 93	28, 45, 68, 88	0
13	a	233/246 (94%)	-0.45	1 (0%) 92 93	28, 44, 66, 84	0
14	N	196/196 (100%)	-0.56	1 (0%) 91 91	27, 39, 68, 95	0
14	b	196/196 (100%)	-0.55	2 (1%) 82 82	28, 41, 69, 104	0
15	c	1/4 (25%)	-0.14	0 100 100	53, 53, 53, 53	0
15	d	1/4 (25%)	-0.48	0 100 100	50, 50, 50, 50	0
All	All	6346/6622 (95%)	-0.32	134 (2%) 63 61	26, 52, 98, 168	0

The worst 5 of 134 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	Q	49	THR	6.8
3	Q	206	LYS	6.3
10	X	1	MET	6.1
10	X	194	ASP	5.8
3	Q	50	LEU	5.7

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

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	N7P	c	1	10/11	0.95	0.14	48,51,55,60	0
15	N7P	d	1	10/11	0.95	0.19	40,44,50,55	0
15	ASJ	d	3	8/8	0.96	0.11	51,54,55,55	0
15	ASJ	c	3	8/8	0.97	0.11	54,57,62,63	0

## 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. 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	CL	U	301	1/1	0.94	0.27	30,30,30,30	0
16	MG	K	301	1/1	0.94	0.15	43,43,43,43	0
16	MG	L	301	1/1	0.95	0.07	64,64,64,64	0
16	MG	N	201	1/1	0.95	0.15	36,36,36,36	0
16	MG	G	301	1/1	0.96	0.08	40,40,40,40	0
17	CL	G	302	1/1	0.96	0.21	30,30,30,30	0
16	MG	Z	301	1/1	0.96	0.12	45,45,45,45	0
16	MG	I	301	1/1	0.96	0.24	59,59,59,59	0
16	MG	I	302	1/1	0.96	0.07	48,48,48,48	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.