



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 29, 2020 – 07:13 am BST

PDB ID : 5FGA  
Title : Yeast 20S proteasome beta5-K33A mutant (propeptide expressed in trans)  
Authors : Huber, E.M.; Groll, M.  
Deposited on : 2015-12-20  
Resolution : 2.70 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

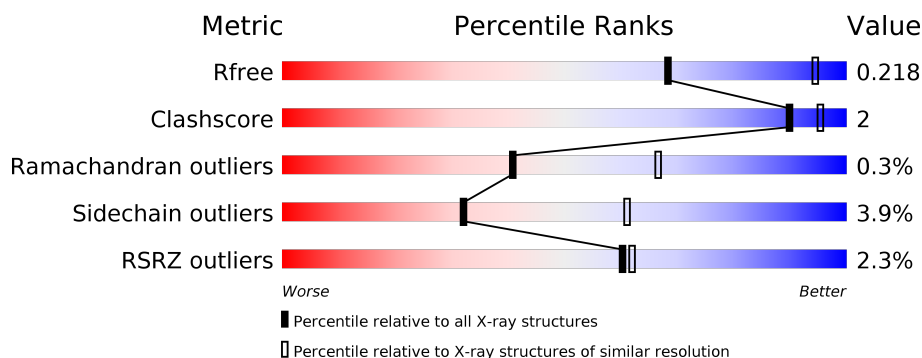
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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>98%</div> <div>•</div> </div>
1	O	250	<div> <div>3%</div> <div>97%</div> <div>•</div> </div>
2	B	258	<div> <div>3%</div> <div>86%</div> <div>7% • 5%</div> </div>
2	P	258	<div> <div>3%</div> <div>86%</div> <div>8% • 5%</div> </div>
3	C	254	<div> <div>6%</div> <div>86%</div> <div>7% • 6%</div> </div>
3	Q	254	<div> <div>7%</div> <div>87%</div> <div>7% • 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	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 17 unique types of molecules in this entry. The entry contains 49871 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
			1640	1042	279	312	7			
11	Y	212	Total	C	N	O	S	0	0	0
			1640	1042	279	312	7			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	33	ALA	LYS	engineered mutation	UNP P30656
Y	33	ALA	LYS	engineered mutation	UNP P30656

- 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	232	Total	C	N	O	S	0	0	0
			1815	1148	311	349	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	K	1	Total Mg 1 1	0	0
15	I	2	Total Mg 2 2	0	0
15	W	1	Total Mg 1 1	0	0
15	Z	1	Total Mg 1 1	0	0
15	N	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 water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	A	20	Total O 20 20	0	0
17	B	14	Total O 14 14	0	0
17	C	20	Total O 20 20	0	0
17	D	16	Total O 16 16	0	0
17	E	10	Total O 10 10	0	0
17	F	18	Total O 18 18	0	0
17	G	23	Total O 23 23	0	0
17	H	25	Total O 25 25	0	0
17	I	16	Total O 16 16	0	0

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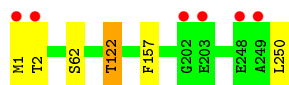
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	J	16	Total 16	O 16	0	0
17	K	17	Total 17	O 17	0	0
17	L	31	Total 31	O 31	0	0
17	M	24	Total 24	O 24	0	0
17	N	22	Total 22	O 22	0	0
17	O	7	Total 7	O 7	0	0
17	P	13	Total 13	O 13	0	0
17	Q	13	Total 13	O 13	0	0
17	R	17	Total 17	O 17	0	0
17	S	5	Total 5	O 5	0	0
17	T	19	Total 19	O 19	0	0
17	U	23	Total 23	O 23	0	0
17	V	18	Total 18	O 18	0	0
17	W	16	Total 16	O 16	0	0
17	X	15	Total 15	O 15	0	0
17	Y	25	Total 25	O 25	0	0
17	Z	19	Total 19	O 19	0	0
17	a	30	Total 30	O 30	0	0
17	b	20	Total 20	O 20	0	0



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

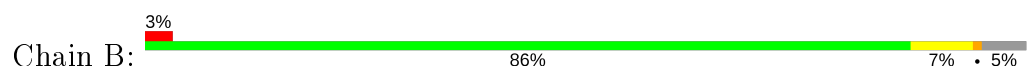
- Molecule 1: Proteasome subunit alpha type-2



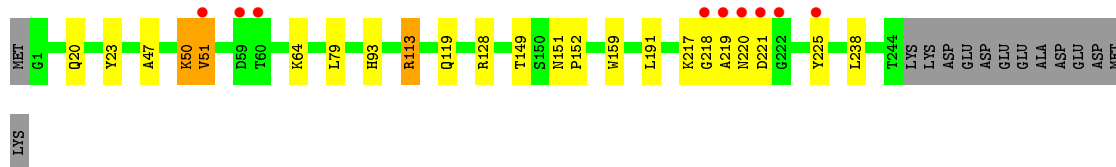
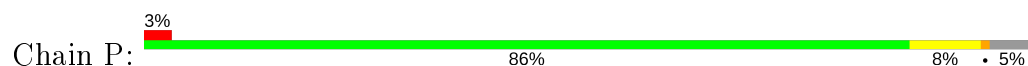
- Molecule 1: Proteasome subunit alpha type-2



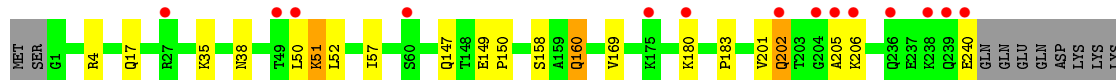
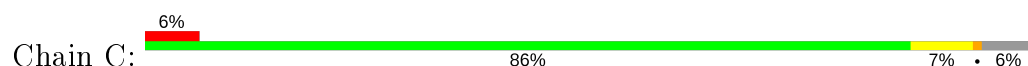
- Molecule 2: Proteasome subunit alpha type-3



- Molecule 2: Proteasome subunit alpha type-3

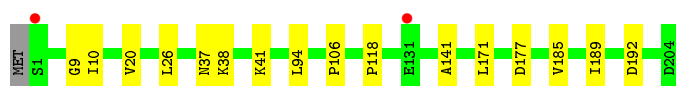


- Molecule 3: Proteasome subunit alpha type-4

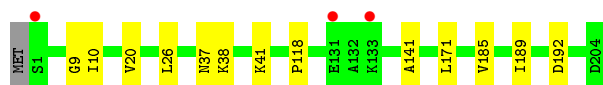


MET	THR	SER	ILE	GLY
T2				
Q19				
Q117				
Y122				
H123				
K139				
L172				
E181				
L198				
E201				
D202				
N203				
Z204				
E205				
Z206				
D207				
W214				
Q240				
T243				
W244				
GLY				
ASP				
ASP				
ASP				
GLU				
ASP				
ASP				
ASP				
SER				
ASN				
VAL				
MET				
SER				
SER				
ASP				
ASP				
GLN				
ALA				
PRO				
VAL				
ALA				

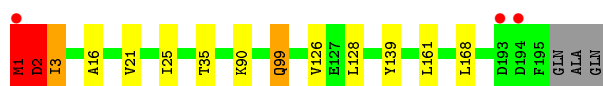
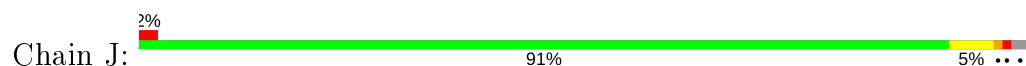




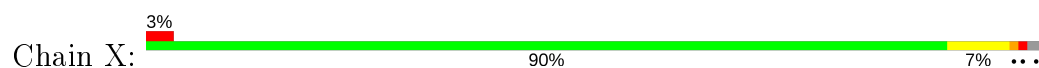
- Molecule 9: Proteasome subunit beta type-3



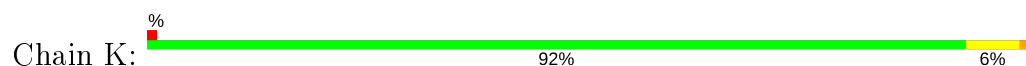
- Molecule 10: Proteasome subunit beta type-4



- Molecule 10: Proteasome subunit beta type-4



- Molecule 11: Proteasome subunit beta type-5



- Molecule 11: Proteasome subunit beta type-5



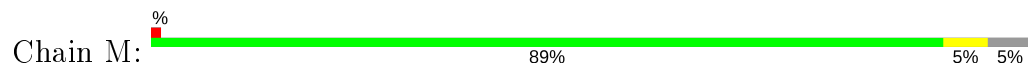
- Molecule 12: Proteasome subunit beta type-6



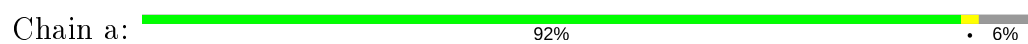
- Molecule 12: Proteasome subunit beta type-6



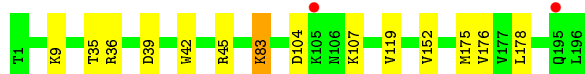
- Molecule 13: Proteasome subunit beta type-7



- Molecule 13: Proteasome subunit beta type-7



- Molecule 14: Proteasome subunit beta type-1



- Molecule 14: Proteasome subunit beta type-1



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	135.35Å 300.50Å 144.44Å 90.00° 113.10° 90.00°	Depositor
Resolution (Å)	15.00 – 2.70 15.00 – 2.70	Depositor EDS
% Data completeness (in resolution range)	98.6 (15.00-2.70) 98.6 (15.00-2.70)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.69 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, $R_{free}$	0.188 , 0.214 0.193 , 0.218	Depositor DCC
$R_{free}$ test set	14192 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	54.0	Xtriage
Anisotropy	0.107	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 38.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	49871	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.57% 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, 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	0.26	0/1952	0.46	0/2642
1	O	0.26	0/1952	0.46	0/2642
2	B	0.27	0/1934	0.49	0/2618
2	P	0.27	0/1934	0.50	0/2618
3	C	0.27	0/1910	0.51	0/2586
3	Q	0.27	0/1910	0.50	0/2586
4	D	0.26	0/1837	0.47	0/2475
4	R	0.26	0/1837	0.47	0/2475
5	E	0.26	0/1800	0.47	0/2433
5	S	0.26	0/1800	0.47	0/2433
6	F	0.27	0/1932	0.45	0/2609
6	T	0.26	0/1932	0.45	0/2609
7	G	0.27	0/1945	0.47	0/2634
7	U	0.26	0/1945	0.47	0/2634
8	H	0.25	0/1750	0.48	0/2373
8	V	0.25	0/1750	0.48	0/2373
9	I	0.27	0/1611	0.50	0/2174
9	W	0.27	0/1611	0.50	0/2174
10	J	0.39	1/1589 (0.1%)	0.76	5/2142 (0.2%)
10	X	0.36	0/1589	0.73	3/2142 (0.1%)
11	K	0.26	0/1677	0.50	0/2270
11	Y	0.26	0/1677	0.50	0/2270
12	L	0.26	0/1795	0.49	0/2420
12	Z	0.26	0/1795	0.49	0/2420
13	M	0.27	0/1855	0.52	0/2514
13	a	0.27	0/1846	0.51	0/2503
14	N	0.25	0/1541	0.49	0/2087
14	b	0.25	0/1541	0.48	0/2087
All	All	0.27	1/50247 (0.0%)	0.51	8/67943 (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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	J	1	MET	SD-CE	8.51	2.25	1.77

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	J	1	MET	CG-SD-CE	15.16	124.46	100.20
10	X	1	MET	CB-CA-C	-15.09	80.22	110.40
10	X	1	MET	CG-SD-CE	13.91	122.46	100.20
10	J	1	MET	CB-CA-C	-12.72	84.96	110.40
10	J	1	MET	CA-CB-CG	-9.42	97.29	113.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
10	J	1	MET	Mainchain
10	J	2	ASP	Peptide
10	X	1	MET	Mainchain

## 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	2	0
1	O	1915	0	1929	4	0
2	B	1904	0	1904	10	0
2	P	1904	0	1904	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	1881	0	1895	7	0
3	Q	1881	0	1895	5	0
4	D	1813	0	1797	5	0
4	R	1813	0	1797	5	0
5	E	1773	0	1775	4	0
5	S	1773	0	1775	4	0
6	F	1892	0	1883	3	0
6	T	1892	0	1883	3	0
7	G	1907	0	1901	6	0
7	U	1907	0	1901	6	0
8	H	1719	0	1719	8	0
8	V	1719	0	1719	14	0
9	I	1581	0	1574	8	0
9	W	1581	0	1574	6	0
10	J	1561	0	1568	13	0
10	X	1561	0	1569	21	0
11	K	1640	0	1587	8	0
11	Y	1640	0	1587	8	0
12	L	1757	0	1711	3	0
12	Z	1757	0	1711	3	0
13	M	1824	0	1832	5	0
13	a	1815	0	1821	0	0
14	N	1512	0	1481	7	0
14	b	1512	0	1481	0	0
15	G	1	0	0	0	0
15	I	2	0	0	0	0
15	K	1	0	0	0	0
15	L	1	0	0	0	0
15	N	1	0	0	0	0
15	W	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	A	20	0	0	0	0
17	B	14	0	0	1	0
17	C	20	0	0	0	0
17	D	16	0	0	0	0
17	E	10	0	0	0	0
17	F	18	0	0	0	0
17	G	23	0	0	0	0
17	H	25	0	0	0	0
17	I	16	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	J	16	0	0	1	0
17	K	17	0	0	1	0
17	L	31	0	0	0	0
17	M	24	0	0	1	0
17	N	22	0	0	0	0
17	O	7	0	0	0	0
17	P	13	0	0	2	0
17	Q	13	0	0	0	0
17	R	17	0	0	0	0
17	S	5	0	0	0	0
17	T	19	0	0	0	0
17	U	23	0	0	0	0
17	V	18	0	0	0	0
17	W	16	0	0	0	0
17	X	15	0	0	1	0
17	Y	25	0	0	1	0
17	Z	19	0	0	0	0
17	a	30	0	0	0	0
17	b	20	0	0	0	0
All	All	49871	0	49102	162	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

The worst 5 of 162 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)
10:J:1:MET:CE	10:J:1:MET:SD	2.25	1.25
10:X:1:MET:O	10:X:1:MET:CE	1.68	1.15
10:X:3:ILE:HD11	10:X:168:LEU:HD13	1.15	1.11
8:V:80:LEU:HG	8:V:113:ILE:HD11	1.33	1.11
13:M:2:GLN:NE2	17:M:301:HOH:O	1.88	1.06

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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%)	34	60
1	O	248/250 (99%)	239 (96%)	8 (3%)	1 (0%)	34	60
2	B	242/258 (94%)	236 (98%)	2 (1%)	4 (2%)	9	23
2	P	242/258 (94%)	236 (98%)	2 (1%)	4 (2%)	9	23
3	C	238/254 (94%)	232 (98%)	3 (1%)	3 (1%)	12	30
3	Q	238/254 (94%)	232 (98%)	3 (1%)	3 (1%)	12	30
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%)	222 (97%)	7 (3%)	0	100	100
5	S	229/234 (98%)	222 (97%)	7 (3%)	0	100	100
6	F	241/288 (84%)	238 (99%)	3 (1%)	0	100	100
6	T	241/288 (84%)	238 (99%)	3 (1%)	0	100	100
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%)	217 (97%)	7 (3%)	0	100	100
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%)	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%)	222 (96%)	9 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	a	230/246 (94%)	221 (96%)	9 (4%)	0	100	100
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	6283/6614 (95%)	6132 (98%)	135 (2%)	16 (0%)	41	66

5 of 16 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	51	VAL
2	B	221	ASP
3	C	202	GLN
2	P	51	VAL
2	P	221	ASP

### 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	82
1	O	209/209 (100%)	205 (98%)	4 (2%)	57	82
2	B	203/216 (94%)	197 (97%)	6 (3%)	41	70
2	P	203/216 (94%)	197 (97%)	6 (3%)	41	70
3	C	212/226 (94%)	202 (95%)	10 (5%)	26	54
3	Q	212/226 (94%)	201 (95%)	11 (5%)	23	49
4	D	194/215 (90%)	184 (95%)	10 (5%)	23	49
4	R	194/215 (90%)	184 (95%)	10 (5%)	23	49
5	E	190/193 (98%)	181 (95%)	9 (5%)	26	54
5	S	190/193 (98%)	181 (95%)	9 (5%)	26	54
6	F	201/239 (84%)	191 (95%)	10 (5%)	24	51
6	T	201/239 (84%)	191 (95%)	10 (5%)	24	51
7	G	206/210 (98%)	196 (95%)	10 (5%)	25	52

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	U	206/210 (98%)	196 (95%)	10 (5%)	25	52
8	H	185/190 (97%)	178 (96%)	7 (4%)	33	62
8	V	185/190 (97%)	178 (96%)	7 (4%)	33	62
9	I	172/173 (99%)	169 (98%)	3 (2%)	60	84
9	W	172/173 (99%)	169 (98%)	3 (2%)	60	84
10	J	173/175 (99%)	168 (97%)	5 (3%)	42	71
10	X	173/175 (99%)	168 (97%)	5 (3%)	42	71
11	K	168/168 (100%)	160 (95%)	8 (5%)	25	53
11	Y	168/168 (100%)	160 (95%)	8 (5%)	25	53
12	L	185/185 (100%)	177 (96%)	8 (4%)	29	57
12	Z	185/185 (100%)	177 (96%)	8 (4%)	29	57
13	M	199/208 (96%)	192 (96%)	7 (4%)	36	65
13	a	198/208 (95%)	192 (97%)	6 (3%)	41	70
14	N	162/162 (100%)	157 (97%)	5 (3%)	40	69
14	b	162/162 (100%)	156 (96%)	6 (4%)	34	63
All	All	5317/5538 (96%)	5112 (96%)	205 (4%)	32	61

5 of 205 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
13	M	70	LEU
3	Q	50	LEU
12	Z	130	SER
13	M	187	ARG
1	O	157	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 108 such sidechains are listed below:

Mol	Chain	Res	Type
13	M	2	GLN
2	P	123	GLN
12	Z	49	ASN
13	M	102	GLN
14	N	161	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 10 ligands modelled in this entry, 10 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 ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

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%)	-0.38	6 (2%) 59 60	40, 52, 85, 126	0
1	O	250/250 (100%)	-0.30	8 (3%) 47 48	46, 62, 105, 133	0
2	B	244/258 (94%)	-0.22	8 (3%) 46 46	40, 60, 101, 155	0
2	P	244/258 (94%)	-0.18	9 (3%) 41 41	48, 65, 106, 153	0
3	C	240/254 (94%)	-0.11	14 (5%) 23 22	41, 64, 124, 154	0
3	Q	240/254 (94%)	0.06	18 (7%) 14 12	49, 74, 154, 181	0
4	D	235/260 (90%)	-0.38	5 (2%) 63 65	44, 64, 96, 137	0
4	R	235/260 (90%)	-0.29	7 (2%) 50 51	47, 67, 106, 141	0
5	E	231/234 (98%)	-0.28	3 (1%) 77 78	47, 65, 101, 143	0
5	S	231/234 (98%)	-0.20	6 (2%) 56 57	49, 72, 109, 150	0
6	F	243/288 (84%)	-0.40	4 (1%) 72 74	42, 57, 107, 130	0
6	T	243/288 (84%)	-0.31	6 (2%) 57 59	41, 66, 121, 148	0
7	G	241/252 (95%)	-0.48	2 (0%) 86 87	36, 53, 87, 134	0
7	U	241/252 (95%)	-0.33	9 (3%) 41 41	44, 59, 88, 132	0
8	H	226/232 (97%)	-0.32	8 (3%) 44 44	38, 52, 87, 154	0
8	V	226/232 (97%)	-0.26	7 (3%) 49 49	43, 55, 92, 169	0
9	I	204/205 (99%)	-0.56	2 (0%) 82 83	40, 52, 79, 97	0
9	W	204/205 (99%)	-0.51	3 (1%) 73 76	43, 54, 83, 104	0
10	J	195/198 (98%)	-0.37	3 (1%) 73 76	40, 55, 81, 128	0
10	X	195/198 (98%)	-0.28	5 (2%) 56 57	36, 59, 84, 145	0
11	K	212/212 (100%)	-0.38	2 (0%) 84 85	40, 57, 79, 100	0
11	Y	212/212 (100%)	-0.44	0 100 100	45, 57, 80, 100	0
12	L	222/222 (100%)	-0.53	1 (0%) 91 92	40, 53, 86, 123	0
12	Z	222/222 (100%)	-0.51	2 (0%) 84 85	41, 53, 85, 122	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	M	233/246 (94%)	-0.60	2 (0%) 84 85	36, 52, 74, 91	0
13	a	232/246 (94%)	-0.54	1 (0%) 92 93	37, 52, 72, 90	0
14	N	196/196 (100%)	-0.60	2 (1%) 82 83	36, 47, 74, 103	0
14	b	196/196 (100%)	-0.59	2 (1%) 82 83	37, 49, 76, 108	0
All	All	6343/6614 (95%)	-0.36	145 (2%) 60 62	36, 58, 100, 181	0

The worst 5 of 145 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	221	ASP	7.5
3	Q	50	LEU	7.1
8	V	224	GLN	7.1
10	X	1	MET	6.7
2	B	219	ALA	6.6

## 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	301	1/1	0.93	0.39	72,72,72,72	0
15	MG	W	301	1/1	0.94	0.48	73,73,73,73	0
15	MG	I	302	1/1	0.95	0.13	57,57,57,57	0
15	MG	Z	301	1/1	0.96	0.40	61,61,61,61	0
15	MG	N	201	1/1	0.97	0.10	49,49,49,49	0
15	MG	K	301	1/1	0.98	0.05	56,56,56,56	0
15	MG	G	301	1/1	0.98	0.09	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
16	CL	U	301	1/1	0.99	0.14	46,46,46,46	0
15	MG	L	301	1/1	0.99	0.05	58,58,58,58	0
16	CL	G	302	1/1	1.00	0.12	39,39,39,39	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.