



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 07:24 am GMT

PDB ID : 5L5A  
Title : Yeast 20S proteasome with human beta5i (1-138; R57T)  
Authors : Groll, M.; Huber, E.M.  
Deposited on : 2016-05-28  
Resolution : 2.40 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

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

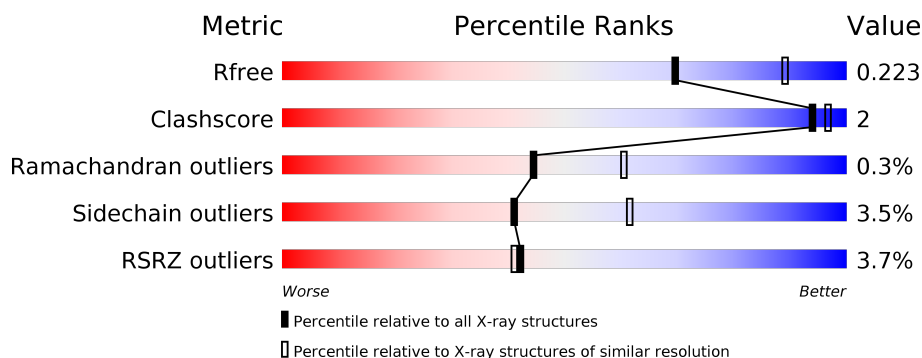
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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))
$R_{free}$	100719	3166 (2.40-2.40)
Clashscore	112137	3674 (2.40-2.40)
Ramachandran outliers	110173	3616 (2.40-2.40)
Sidechain outliers	110143	3617 (2.40-2.40)
RSRZ outliers	101464	3195 (2.40-2.40)

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

Mol	Chain	Length	Quality of chain
1	A	250	<div> <div>4%</div> <div>98%</div> <div>•</div> </div>
1	O	250	<div> <div>4%</div> <div>96%</div> <div>•</div> </div>
2	B	258	<div> <div>6%</div> <div>86%</div> <div>8% • 5%</div> </div>
2	P	258	<div> <div>5%</div> <div>86%</div> <div>7% • 5%</div> </div>
3	C	254	<div> <div>9%</div> <div>86%</div> <div>7% • 6%</div> </div>
3	Q	254	<div> <div>12%</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	211	
11	Y	211	
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 50851 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			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	X	195	Total	C	N	O	S	0	0	0
			1561	992	264	299	6			

- Molecule 11 is a protein called Proteasome subunit beta type-8, Proteasome subunit beta type-5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	211	Total	C	N	O	S	0	0	0
			1636	1033	279	312	12			
11	Y	211	Total	C	N	O	S	0	0	0
			1636	1033	279	312	12			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	57	THR	ARG	engineered mutation	UNP P28062
Y	57	THR	ARG	engineered mutation	UNP P28062

- 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	1	0
			1832	1159	315	351	7			
13	a	233	Total	C	N	O	S	0	1	0
			1835	1160	316	352	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 1	Mg 1	0	0
15	J	1	Total 1	Mg 1	0	0
15	K	2	Total 2	Mg 2	0	0
15	H	1	Total 1	Mg 1	0	0
15	I	2	Total 2	Mg 2	0	0
15	Z	1	Total 1	Mg 1	0	0
15	N	1	Total 1	Mg 1	0	0
15	L	1	Total 1	Mg 1	0	0

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

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

- Molecule 17 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	A	68	Total 68	O 68	0	0
17	B	44	Total 44	O 44	0	0
17	C	39	Total 39	O 39	0	0
17	D	35	Total 35	O 35	0	0
17	E	25	Total 25	O 25	0	0
17	F	49	Total 49	O 49	0	0
17	G	66	Total 66	O 66	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	H	60	Total 60	O 60	0	0
17	I	67	Total 67	O 67	0	0
17	J	55	Total 55	O 55	0	0
17	K	39	Total 39	O 39	0	0
17	L	68	Total 68	O 68	0	0
17	M	86	Total 86	O 86	0	0
17	N	58	Total 58	O 58	0	0
17	O	35	Total 35	O 35	0	0
17	P	33	Total 33	O 33	0	0
17	Q	24	Total 24	O 24	0	0
17	R	30	Total 30	O 30	0	0
17	S	27	Total 27	O 27	0	0
17	T	38	Total 38	O 38	0	0
17	U	75	Total 75	O 75	0	0
17	V	55	Total 55	O 55	0	0
17	W	71	Total 71	O 71	0	0
17	X	54	Total 54	O 54	0	0
17	Y	45	Total 45	O 45	0	0
17	Z	72	Total 72	O 72	0	0
17	a	81	Total 81	O 81	0	0
17	b	64	Total 64	O 64	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.

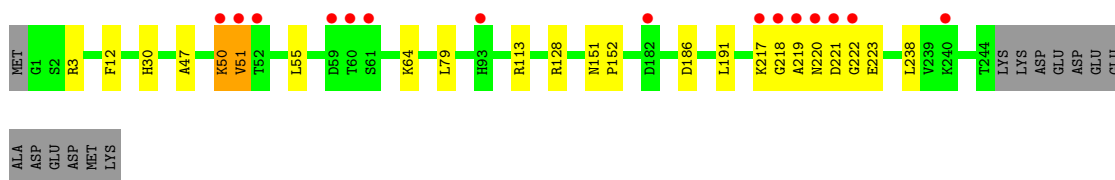
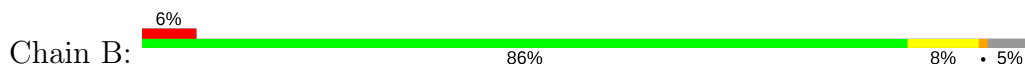
- Molecule 1: Proteasome subunit alpha type-2



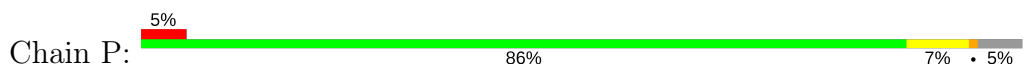
- Molecule 1: Proteasome subunit alpha type-2



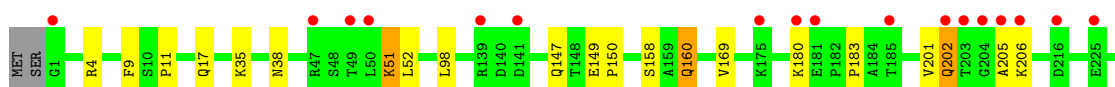
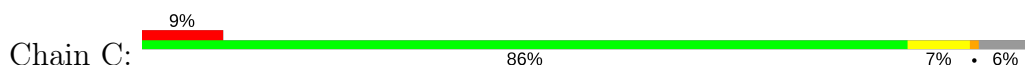
- Molecule 2: Proteasome subunit alpha type-3

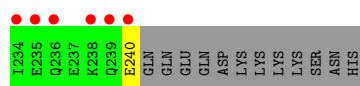


- Molecule 2: Proteasome subunit alpha type-3

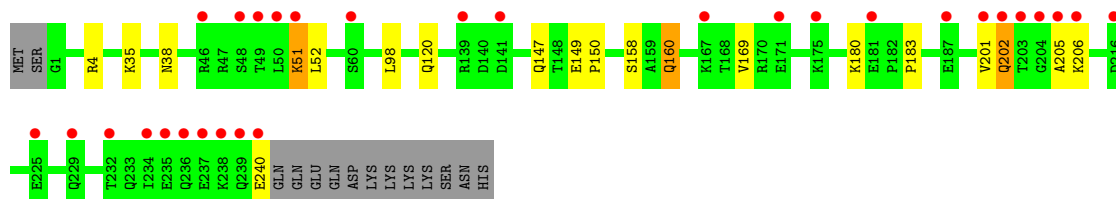
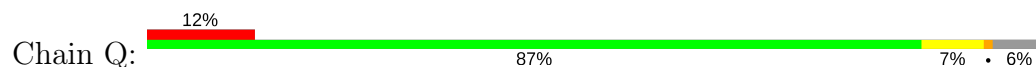


- Molecule 3: Proteasome subunit alpha type-4

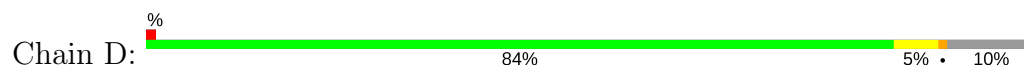




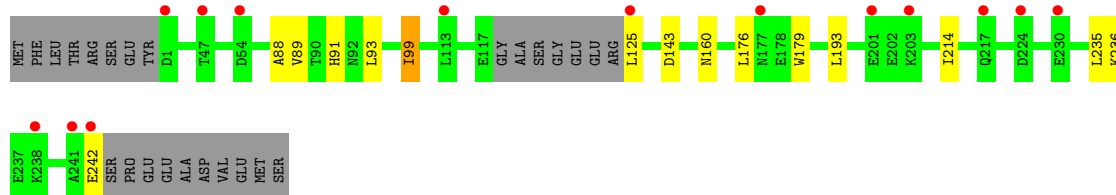
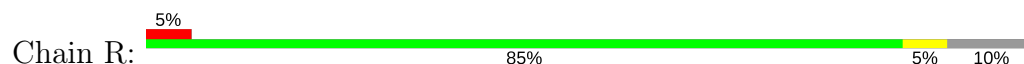
• Molecule 3: Proteasome subunit alpha type-4



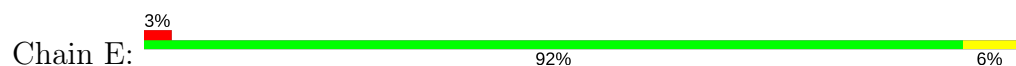
• Molecule 4: Proteasome subunit alpha type-5



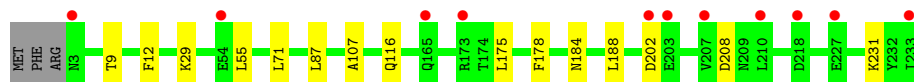
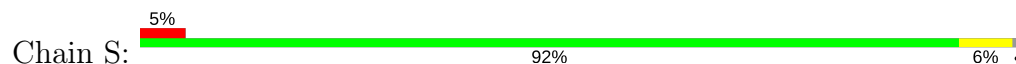
• Molecule 4: Proteasome subunit alpha type-5



• Molecule 5: Proteasome subunit alpha type-6



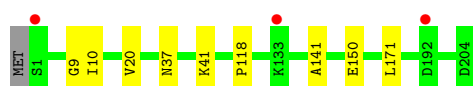
• Molecule 5: Proteasome subunit alpha type-6



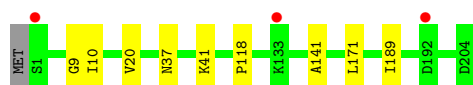
• Molecule 6: Probable proteasome subunit alpha type-7



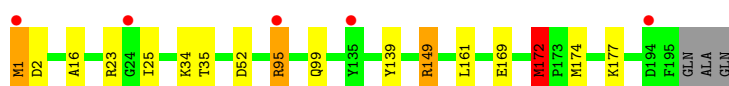
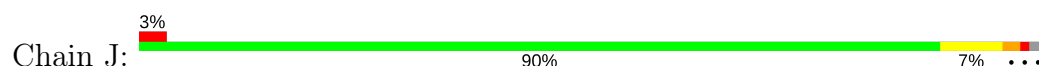




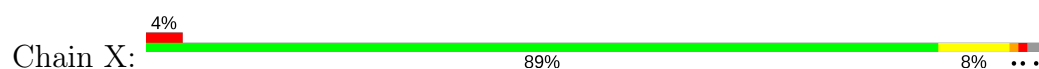
- Molecule 9: Proteasome subunit beta type-3



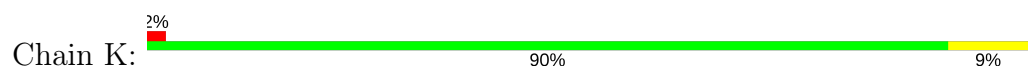
- Molecule 10: Proteasome subunit beta type-4



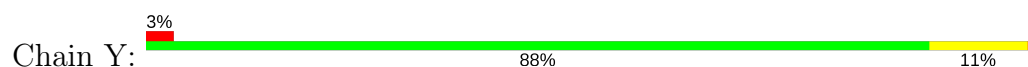
- Molecule 10: Proteasome subunit beta type-4



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



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



- Molecule 12: Proteasome subunit beta type-6

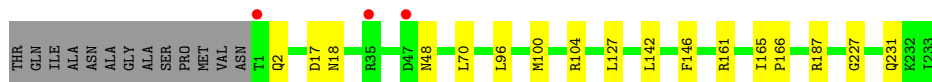
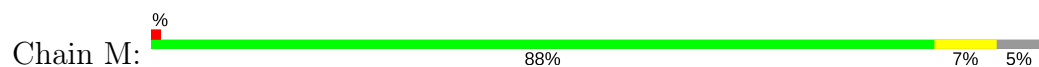


- Molecule 12: Proteasome subunit beta type-6

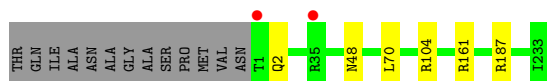




- Molecule 13: Proteasome subunit beta type-7



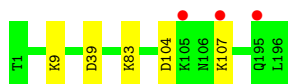
- Molecule 13: Proteasome subunit beta type-7



- 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, $\alpha$ , $\beta$ , $\gamma$	135.14Å 301.15Å 145.06Å 90.00° 112.57° 90.00°	Depositor
Resolution (Å)	15.00 – 2.40 15.00 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.2 (15.00-2.40) 99.2 (15.00-2.40)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.05 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, $R_{free}$	0.200 , 0.219 0.204 , 0.223	Depositor DCC
$R_{free}$ test set	20515 reflections (5.26%)	DCC
Wilson B-factor (Å <sup>2</sup> )	46.9	Xtriage
Anisotropy	0.122	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 38.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	50851	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.39% 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	0.27	0/1952	0.46	0/2642
1	O	0.27	0/1952	0.46	0/2642
2	B	0.27	0/1934	0.49	0/2618
2	P	0.27	0/1934	0.49	0/2618
3	C	0.27	0/1910	0.51	0/2586
3	Q	0.28	0/1910	0.51	0/2586
4	D	0.27	0/1837	0.47	0/2475
4	R	0.27	0/1837	0.47	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	0.28	0/1945	0.48	0/2634
7	U	0.28	0/1945	0.47	0/2634
8	H	0.40	2/1761 (0.1%)	0.56	2/2388 (0.1%)
8	V	0.30	0/1750	0.47	0/2373
9	I	0.28	0/1611	0.49	0/2174
9	W	0.28	0/1611	0.49	0/2174
10	J	0.38	0/1589	1.01	8/2142 (0.4%)
10	X	0.34	0/1589	0.97	6/2142 (0.3%)
11	K	0.35	0/1673	0.52	0/2259
11	Y	0.38	0/1673	0.54	0/2259
12	L	0.29	0/1795	0.47	0/2420
12	Z	0.35	0/1795	0.48	0/2420
13	M	0.38	0/1866	0.55	0/2528
13	a	0.27	0/1866	0.51	0/2528
14	N	0.28	0/1541	0.48	0/2087
14	b	0.27	0/1541	0.48	0/2087
All	All	0.30	2/50281 (0.0%)	0.53	16/67975 (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	2
All	All	0	4

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	5.99	1.68	1.52
8	H	114[B]	HIS	CA-C	5.99	1.68	1.52

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	J	149	ARG	NE-CZ-NH1	-21.12	109.74	120.30
10	J	95	ARG	NE-CZ-NH2	-20.61	110.00	120.30
10	X	149	ARG	NE-CZ-NH2	-20.09	110.25	120.30
10	X	95	ARG	NE-CZ-NH1	-19.31	110.65	120.30
10	X	95	ARG	NE-CZ-NH2	16.04	128.32	120.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

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

## 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1915	0	1929	2	0
1	O	1915	0	1929	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1904	0	1904	11	0
2	P	1904	0	1904	9	0
3	C	1881	0	1895	8	0
3	Q	1881	0	1895	6	0
4	D	1813	0	1797	9	0
4	R	1813	0	1797	7	0
5	E	1773	0	1775	5	0
5	S	1773	0	1775	3	0
6	F	1892	0	1883	4	0
6	T	1892	0	1883	4	0
7	G	1907	0	1901	5	0
7	U	1907	0	1901	6	0
8	H	1726	0	1726	13	0
8	V	1719	0	1719	4	0
9	I	1581	0	1574	4	0
9	W	1581	0	1574	4	0
10	J	1561	0	1569	11	0
10	X	1561	0	1569	14	0
11	K	1636	0	1575	14	0
11	Y	1636	0	1575	18	0
12	L	1757	0	1711	2	0
12	Z	1757	0	1711	3	0
13	M	1832	0	1845	5	0
13	a	1835	0	1844	0	0
14	N	1512	0	1481	2	0
14	b	1512	0	1481	0	0
15	G	1	0	0	0	0
15	H	1	0	0	0	0
15	I	2	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	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	68	0	0	0	0
17	B	44	0	0	0	0
17	C	39	0	0	0	0
17	D	35	0	0	0	0
17	E	25	0	0	0	0
17	F	49	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	G	66	0	0	0	0
17	H	60	0	0	0	0
17	I	67	0	0	0	0
17	J	55	0	0	0	0
17	K	39	0	0	0	0
17	L	68	0	0	0	0
17	M	86	0	0	0	0
17	N	58	0	0	0	0
17	O	35	0	0	0	0
17	P	33	0	0	1	0
17	Q	24	0	0	0	0
17	R	30	0	0	1	0
17	S	27	0	0	0	0
17	T	38	0	0	0	0
17	U	75	0	0	0	0
17	V	55	0	0	0	0
17	W	71	0	0	0	0
17	X	54	0	0	0	0
17	Y	45	0	0	0	0
17	Z	72	0	0	0	0
17	a	81	0	0	0	0
17	b	64	0	0	0	0
All	All	50851	0	49122	149	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 149 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)
11:Y:18:SER:OG	11:Y:30:ARG:HA	1.73	0.88
8:H:53:GLU:O	8:H:57:GLN:HG2	1.79	0.82
10:J:23:ARG:NH2	11:K:119:THR:OG1	2.15	0.80
10:J:174:MET:SD	10:X:174:MET:SD	2.80	0.80
4:R:89:VAL:HG12	11:Y:61:LYS:HG3	1.65	0.78

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%)	38	54
1	O	248/250 (99%)	239 (96%)	8 (3%)	1 (0%)	38	54
2	B	242/258 (94%)	234 (97%)	4 (2%)	4 (2%)	11	13
2	P	242/258 (94%)	234 (97%)	4 (2%)	4 (2%)	11	13
3	C	238/254 (94%)	232 (98%)	3 (1%)	3 (1%)	14	19
3	Q	238/254 (94%)	232 (98%)	3 (1%)	3 (1%)	14	19
4	D	231/260 (89%)	228 (99%)	3 (1%)	0	100	100
4	R	231/260 (89%)	228 (99%)	3 (1%)	0	100	100
5	E	229/234 (98%)	224 (98%)	5 (2%)	0	100	100
5	S	229/234 (98%)	224 (98%)	5 (2%)	0	100	100
6	F	241/288 (84%)	236 (98%)	5 (2%)	0	100	100
6	T	241/288 (84%)	236 (98%)	5 (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	225/232 (97%)	220 (98%)	5 (2%)	0	100	100
8	V	224/232 (97%)	219 (98%)	5 (2%)	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%)	191 (99%)	2 (1%)	0	100	100
10	X	193/198 (98%)	191 (99%)	2 (1%)	0	100	100
11	K	209/211 (99%)	201 (96%)	8 (4%)	0	100	100
11	Y	209/211 (99%)	201 (96%)	8 (4%)	0	100	100
12	L	220/222 (99%)	216 (98%)	4 (2%)	0	100	100
12	Z	220/222 (99%)	216 (98%)	4 (2%)	0	100	100
13	M	232/246 (94%)	225 (97%)	7 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	a	232/246 (94%)	225 (97%)	7 (3%)	0	100	100
14	N	194/196 (99%)	189 (97%)	5 (3%)	0	100	100
14	b	194/196 (99%)	189 (97%)	5 (3%)	0	100	100
All	All	6285/6612 (95%)	6134 (98%)	135 (2%)	16 (0%)	44	60

5 of 16 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%)	205 (98%)	4 (2%)	62	80
1	O	209/209 (100%)	205 (98%)	4 (2%)	62	80
2	B	203/216 (94%)	196 (97%)	7 (3%)	42	63
2	P	203/216 (94%)	196 (97%)	7 (3%)	42	63
3	C	212/226 (94%)	202 (95%)	10 (5%)	30	48
3	Q	212/226 (94%)	202 (95%)	10 (5%)	30	48
4	D	194/215 (90%)	185 (95%)	9 (5%)	31	49
4	R	194/215 (90%)	185 (95%)	9 (5%)	31	49
5	E	190/193 (98%)	180 (95%)	10 (5%)	26	42
5	S	190/193 (98%)	180 (95%)	10 (5%)	26	42
6	F	201/239 (84%)	191 (95%)	10 (5%)	28	45
6	T	201/239 (84%)	191 (95%)	10 (5%)	28	45
7	G	206/210 (98%)	197 (96%)	9 (4%)	33	51

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	U	206/210 (98%)	197 (96%)	9 (4%)	33	51
8	H	186/190 (98%)	179 (96%)	7 (4%)	38	58
8	V	185/190 (97%)	181 (98%)	4 (2%)	57	76
9	I	172/173 (99%)	170 (99%)	2 (1%)	75	88
9	W	172/173 (99%)	170 (99%)	2 (1%)	75	88
10	J	173/175 (99%)	168 (97%)	5 (3%)	48	68
10	X	173/175 (99%)	169 (98%)	4 (2%)	56	75
11	K	170/170 (100%)	162 (95%)	8 (5%)	30	48
11	Y	170/170 (100%)	162 (95%)	8 (5%)	30	48
12	L	185/185 (100%)	182 (98%)	3 (2%)	68	83
12	Z	185/185 (100%)	182 (98%)	3 (2%)	68	83
13	M	200/208 (96%)	193 (96%)	7 (4%)	41	61
13	a	200/208 (96%)	194 (97%)	6 (3%)	46	67
14	N	162/162 (100%)	157 (97%)	5 (3%)	45	66
14	b	162/162 (100%)	157 (97%)	5 (3%)	45	66
All	All	5325/5542 (96%)	5138 (96%)	187 (4%)	41	61

5 of 187 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
13	M	2	GLN
2	P	186	ASP
11	Y	147	LEU
13	M	104	ARG
14	N	104	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 104 such sidechains are listed below:

Mol	Chain	Res	Type
12	L	95	HIS
2	P	119	GLN
12	Z	3	ASN
12	L	158	ASN
13	M	213	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 12 ligands modelled in this entry, 12 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%)	-0.23	10 (4%)	39 38	31, 45, 82, 119	0
1	O	250/250 (100%)	-0.12	11 (4%)	35 33	37, 53, 97, 128	0
2	B	244/258 (94%)	-0.00	15 (6%)	22 20	32, 51, 94, 140	0
2	P	244/258 (94%)	0.01	14 (5%)	24 23	36, 54, 96, 141	0
3	C	240/254 (94%)	0.33	23 (9%)	9 8	32, 58, 125, 163	0
3	Q	240/254 (94%)	0.42	30 (12%)	4 4	28, 64, 146, 188	0
4	D	235/260 (90%)	-0.14	3 (1%)	77 75	39, 55, 88, 131	0
4	R	235/260 (90%)	0.01	14 (5%)	23 21	43, 61, 98, 134	0
5	E	231/234 (98%)	-0.12	8 (3%)	44 43	37, 55, 94, 144	0
5	S	231/234 (98%)	0.04	11 (4%)	31 30	42, 64, 102, 143	0
6	F	243/288 (84%)	-0.20	11 (4%)	34 32	31, 49, 98, 126	0
6	T	243/288 (84%)	-0.11	9 (3%)	42 41	34, 58, 111, 141	0
7	G	241/252 (95%)	-0.31	7 (2%)	52 50	25, 45, 80, 132	0
7	U	241/252 (95%)	-0.13	9 (3%)	42 41	35, 50, 82, 121	0
8	H	226/232 (97%)	-0.18	8 (3%)	44 43	29, 45, 77, 137	0
8	V	226/232 (97%)	-0.12	8 (3%)	44 43	32, 47, 78, 146	0
9	I	204/205 (99%)	-0.47	3 (1%)	74 72	29, 41, 70, 92	0
9	W	204/205 (99%)	-0.45	3 (1%)	74 72	31, 43, 73, 95	0
10	J	195/198 (98%)	-0.25	5 (2%)	56 54	25, 45, 69, 121	0
10	X	195/198 (98%)	-0.25	7 (3%)	43 42	29, 46, 72, 131	0
11	K	211/211 (100%)	0.06	4 (1%)	67 64	36, 54, 86, 108	0
11	Y	211/211 (100%)	0.09	6 (2%)	53 51	37, 57, 89, 116	0
12	L	222/222 (100%)	-0.32	2 (0%)	84 82	31, 45, 78, 114	0
12	Z	222/222 (100%)	-0.29	4 (1%)	69 66	28, 48, 81, 120	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	M	233/246 (94%)	-0.49	3 (1%) 77 75	28, 43, 64, 81	0
13	a	233/246 (94%)	-0.40	2 (0%) 84 82	29, 45, 65, 82	0
14	N	196/196 (100%)	-0.44	2 (1%) 82 80	24, 40, 66, 96	0
14	b	196/196 (100%)	-0.40	3 (1%) 74 72	31, 41, 67, 101	0
All	All	6342/6612 (95%)	-0.15	235 (3%) 42 41	24, 50, 92, 188	0

The worst 5 of 235 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	P	219	ALA	10.5
8	V	224	GLN	9.3
2	P	51	VAL	8.3
12	L	174	TYR	7.8
9	I	1	SER	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
15	MG	I	301	1/1	0.93	0.15	1.40	51,51,51,51	0
15	MG	Z	301	1/1	0.94	0.15	0.65	60,60,60,60	0
15	MG	G	301	1/1	0.99	0.11	-0.07	39,39,39,39	0
15	MG	J	201	1/1	0.98	0.10	-0.47	52,52,52,52	0
15	MG	L	301	1/1	0.97	0.07	-1.82	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
15	MG	N	201	1/1	0.99	0.05	-2.10	38,38,38,38	0
15	MG	K	301	1/1	0.93	0.06	-2.28	46,46,46,46	0
15	MG	I	302	1/1	0.97	0.05	-3.25	41,41,41,41	0
15	MG	K	302	1/1	0.92	0.39	-	64,64,64,64	0
16	CL	U	301	1/1	0.99	0.14	-	30,30,30,30	0
15	MG	H	301	1/1	0.93	0.09	-	57,57,57,57	0
16	CL	G	302	1/1	0.99	0.07	-	30,30,30,30	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.