



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 1, 2025 – 10:35 am BST

PDB ID : 9QCF / pdb_00009qcf
Title : Yeast 20S proteasome mutant: beta1_G128V
Authors : Huber, E.M.; Heinemeyer, W.; Groll, M.
Deposited on : 2025-03-04
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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.46

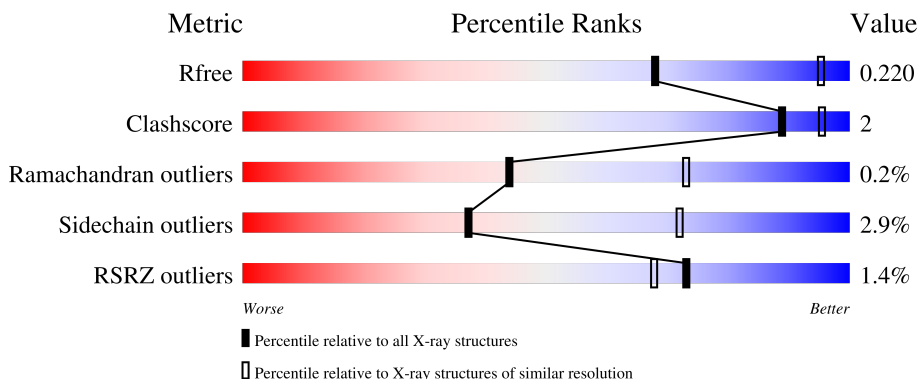
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	2335 (2.90-2.90)
Clashscore	180529	2564 (2.90-2.90)
Ramachandran outliers	177936	2514 (2.90-2.90)
Sidechain outliers	177891	2516 (2.90-2.90)
RSRZ outliers	164620	2337 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 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>0%</div> <div>98%</div> <div>0%</div> </div>
1	O	250	<div> <div>0%</div> <div>98%</div> <div>0%</div> </div>
2	B	258	<div> <div>2%</div> <div>90%</div> <div>5%</div> </div>
2	P	258	<div> <div>2%</div> <div>90%</div> <div>5%</div> </div>
3	C	254	<div> <div>2%</div> <div>91%</div> <div>6%</div> </div>

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Mol	Chain	Length	Quality of chain
3	Q	254	
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	215	
14	b	215	

2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 49433 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	222	Total	C	N	O	S	0	0	0
			1684	1061	293	323	7			
8	V	222	Total	C	N	O	S	0	0	0
			1684	1061	293	323	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
			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	191	Total	C	N	O	S	0	0	0
			1474	931	246	291	6			
14	b	191	Total	C	N	O	S	0	0	0
			1474	931	246	291	6			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
N	128	VAL	GLY	conflict	UNP P38624
b	128	VAL	GLY	conflict	UNP P38624

- Molecule 15 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 16 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

- Molecule 17 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	A	2	Total O 2 2	0	0
17	B	8	Total O 8 8	0	0
17	C	9	Total O 9 9	0	0
17	D	3	Total O 3 3	0	0
17	E	4	Total O 4 4	0	0
17	F	6	Total O 6 6	0	0
17	G	6	Total O 6 6	0	0

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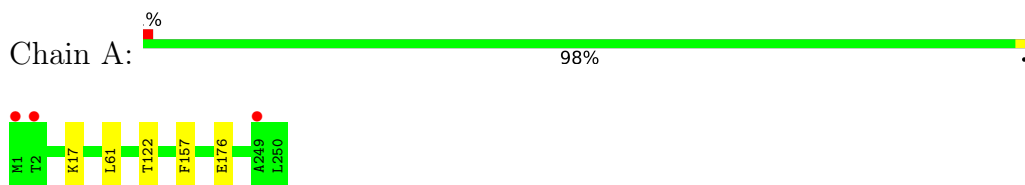
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	H	9	Total O 9 9	0	0
17	I	4	Total O 4 4	0	0
17	J	8	Total O 8 8	0	0
17	K	12	Total O 12 12	0	0
17	L	11	Total O 11 11	0	0
17	M	10	Total O 10 10	0	0
17	N	8	Total O 8 8	0	0
17	O	3	Total O 3 3	0	0
17	P	8	Total O 8 8	0	0
17	Q	6	Total O 6 6	0	0
17	R	6	Total O 6 6	0	0
17	S	5	Total O 5 5	0	0
17	T	4	Total O 4 4	0	0
17	U	7	Total O 7 7	0	0
17	V	11	Total O 11 11	0	0
17	W	5	Total O 5 5	0	0
17	X	9	Total O 9 9	0	0
17	Y	12	Total O 12 12	0	0
17	Z	12	Total O 12 12	0	0
17	a	9	Total O 9 9	0	0
17	b	4	Total O 4 4	0	0

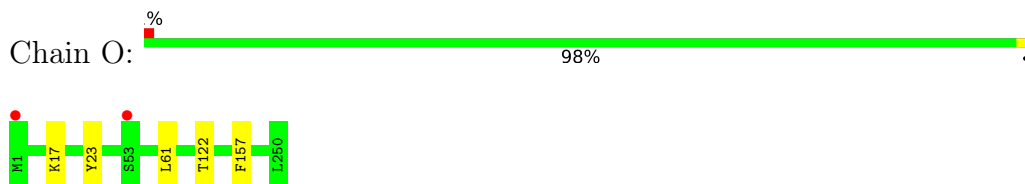
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

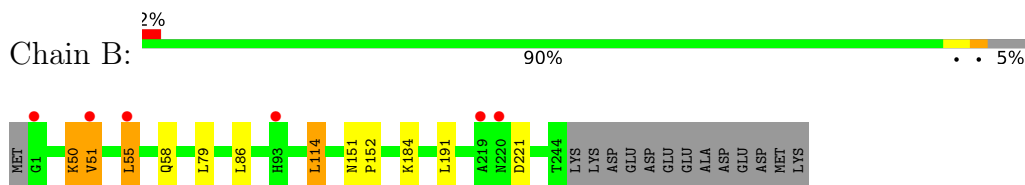
- Molecule 1: Proteasome subunit alpha type-2



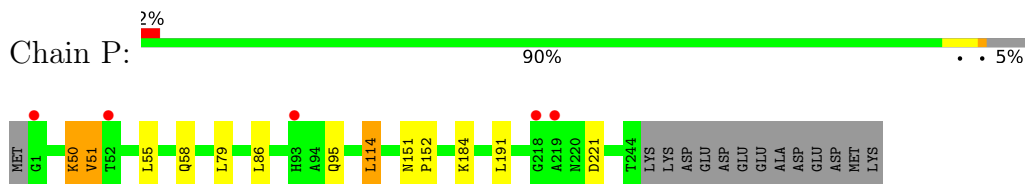
- Molecule 1: Proteasome subunit alpha type-2



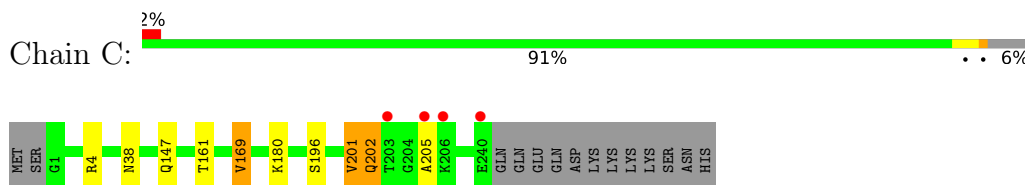
- Molecule 2: Proteasome subunit alpha type-3



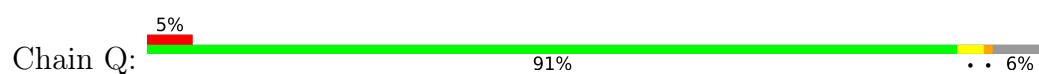
- Molecule 2: Proteasome subunit alpha type-3



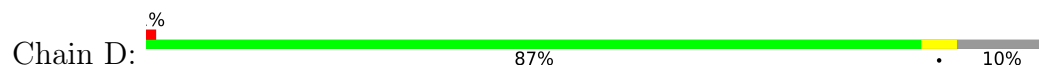
- Molecule 3: Proteasome subunit alpha type-4



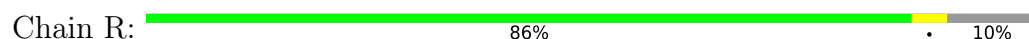
- Molecule 3: Proteasome subunit alpha type-4



- Molecule 4: Proteasome subunit alpha type-5



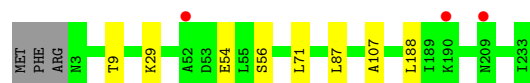
- Molecule 4: Proteasome subunit alpha type-5



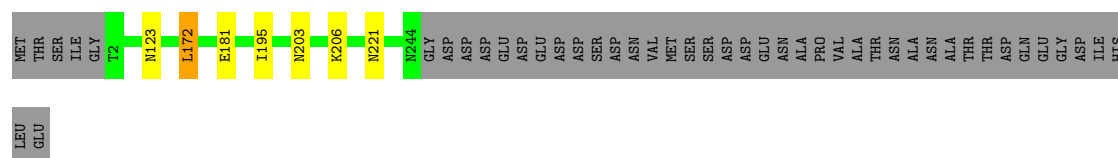
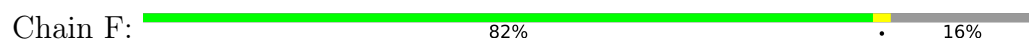
- Molecule 5: Proteasome subunit alpha type-6



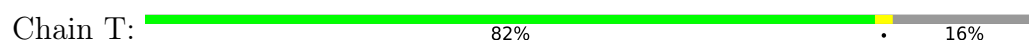
- Molecule 5: Proteasome subunit alpha type-6



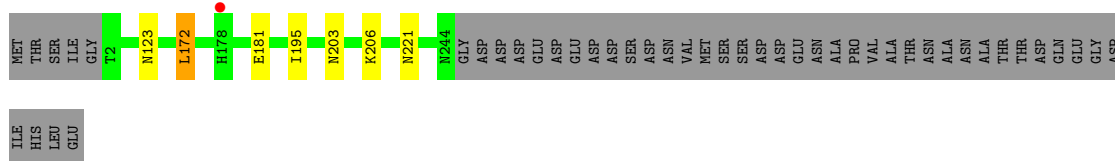
- Molecule 6: Probable proteasome subunit alpha type-7



- Molecule 6: Probable proteasome subunit alpha type-7



LEU
GLU



- Molecule 7: Proteasome subunit alpha type-1

Chain G: 90% 5% .



- Molecule 7: Proteasome subunit alpha type-1

Chain U: 90% 5% .



- Molecule 8: Proteasome subunit beta type-2

Chain H: 92% . .



- Molecule 8: Proteasome subunit beta type-2

Chain V: 92% . .



- Molecule 9: Proteasome subunit beta type-3

Chain I: 93% 7%

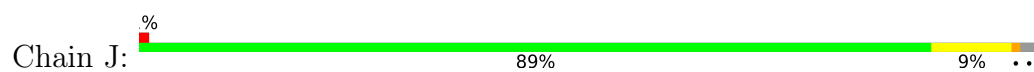


- Molecule 9: Proteasome subunit beta type-3

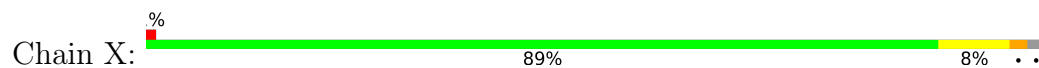
Chain W: 92% 8%



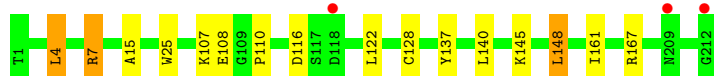
- Molecule 10: Proteasome subunit beta type-4



- Molecule 10: Proteasome subunit beta type-4



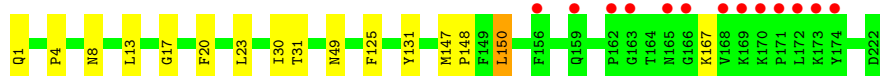
- Molecule 11: Proteasome subunit beta type-5



- Molecule 11: Proteasome subunit beta type-5



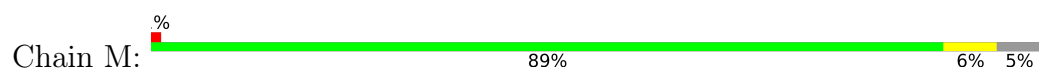
- Molecule 12: Proteasome subunit beta type-6



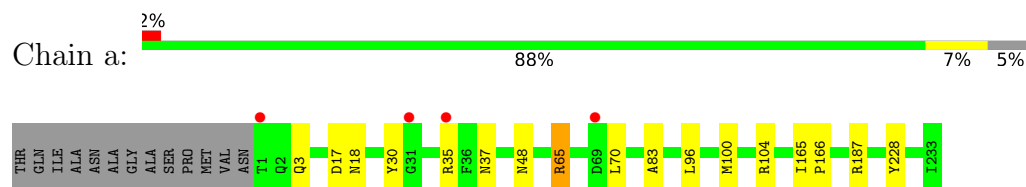
- Molecule 12: Proteasome subunit beta type-6



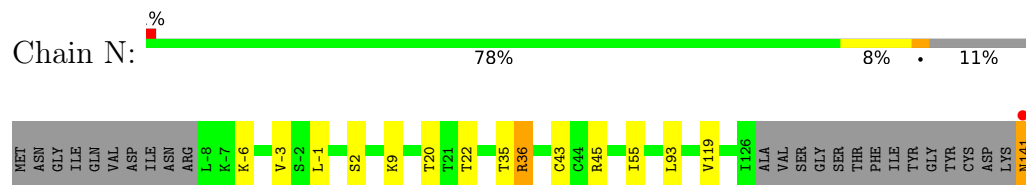
- Molecule 13: Proteasome subunit beta type-7



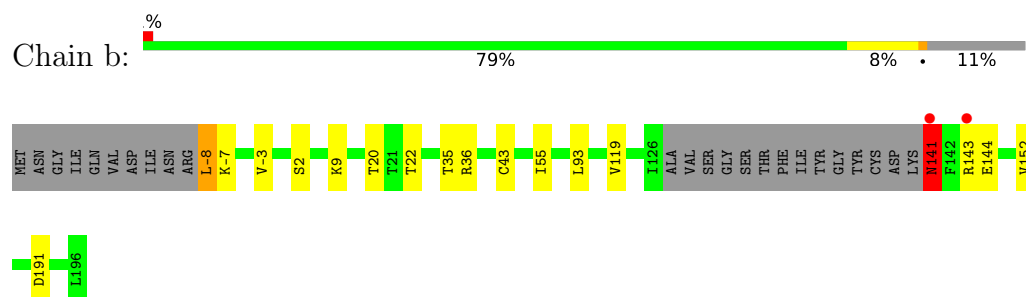
- Molecule 13: Proteasome subunit beta type-7



- 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, α , β , γ	134.91Å 301.57Å 144.43Å 90.00° 112.99° 90.00°	Depositor
Resolution (Å)	15.00 – 2.90 15.00 – 2.90	Depositor EDS
% Data completeness (in resolution range)	97.5 (15.00-2.90) 96.8 (15.00-2.90)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.66 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.188 , 0.214 0.194 , 0.220	Depositor DCC
R_{free} test set	11327 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	61.6	Xtriage
Anisotropy	0.065	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 57.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	49433	wwPDB-VP
Average B, all atoms (Å ²)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.26% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: CL, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.39	0/1952	0.68	0/2642
1	O	0.39	0/1952	0.68	0/2642
2	B	0.39	0/1934	0.66	0/2618
2	P	0.39	0/1934	0.66	0/2618
3	C	0.39	0/1910	0.70	1/2586 (0.0%)
3	Q	0.39	0/1910	0.70	1/2586 (0.0%)
4	D	0.38	0/1837	0.65	0/2475
4	R	0.38	0/1837	0.65	0/2475
5	E	0.38	0/1800	0.66	0/2433
5	S	0.38	0/1800	0.66	0/2433
6	F	0.40	0/1932	0.71	0/2609
6	T	0.39	0/1932	0.71	0/2609
7	G	0.38	0/1945	0.66	0/2634
7	U	0.39	0/1945	0.66	0/2634
8	H	0.35	0/1715	0.68	0/2326
8	V	0.35	0/1715	0.68	0/2326
9	I	0.36	0/1611	0.72	0/2174
9	W	0.36	0/1611	0.72	0/2174
10	J	0.48	0/1589	0.77	0/2142
10	X	0.47	0/1589	0.73	0/2142
11	K	0.35	0/1681	0.69	0/2274
11	Y	0.35	0/1681	0.69	0/2274
12	L	0.35	0/1795	0.69	0/2420
12	Z	0.35	0/1795	0.69	0/2420
13	M	0.37	0/1855	0.73	1/2514 (0.0%)
13	a	0.37	0/1855	0.73	0/2514
14	N	0.37	0/1499	0.70	0/2027
14	b	0.36	0/1499	0.73	1/2027 (0.0%)
All	All	0.38	0/50110	0.69	4/67748 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	201	VAL	N-CA-C	5.46	115.90	110.23
3	Q	201	VAL	N-CA-C	5.39	115.84	110.23
14	b	141	ASN	CB-CA-C	5.32	120.22	110.10
13	M	10	SER	N-CA-C	5.05	117.42	110.35

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	1	0
2	B	1904	0	1904	4	0
2	P	1904	0	1904	4	0
3	C	1881	0	1895	4	0
3	Q	1881	0	1895	4	0
4	D	1813	0	1797	1	0
4	R	1813	0	1797	2	0
5	E	1773	0	1775	1	0
5	S	1773	0	1775	2	0
6	F	1892	0	1883	1	0
6	T	1892	0	1883	1	0
7	G	1907	0	1901	4	0
7	U	1907	0	1901	5	0
8	H	1684	0	1688	3	0
8	V	1684	0	1688	3	0
9	I	1581	0	1574	7	0
9	W	1581	0	1574	9	0
10	J	1561	0	1569	20	0
10	X	1561	0	1569	15	0
11	K	1644	0	1595	20	0
11	Y	1644	0	1595	21	0
12	L	1757	0	1711	7	0
12	Z	1757	0	1711	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	M	1824	0	1832	17	0
13	a	1824	0	1832	10	0
14	N	1474	0	1463	14	0
14	b	1474	0	1463	9	0
15	G	2	0	0	0	0
15	I	1	0	0	0	0
15	K	1	0	0	0	0
15	N	1	0	0	0	0
15	V	1	0	0	0	0
15	Y	1	0	0	0	0
15	Z	1	0	0	0	0
16	G	1	0	0	0	0
16	N	1	0	0	0	0
16	U	1	0	0	0	0
16	b	1	0	0	0	0
17	A	2	0	0	0	0
17	B	8	0	0	0	0
17	C	9	0	0	0	0
17	D	3	0	0	0	0
17	E	4	0	0	0	0
17	F	6	0	0	0	0
17	G	6	0	0	0	0
17	H	9	0	0	0	0
17	I	4	0	0	0	0
17	J	8	0	0	0	0
17	K	12	0	0	0	0
17	L	11	0	0	0	0
17	M	10	0	0	0	0
17	N	8	0	0	1	0
17	O	3	0	0	0	0
17	P	8	0	0	0	0
17	Q	6	0	0	0	0
17	R	6	0	0	0	0
17	S	5	0	0	0	0
17	T	4	0	0	0	0
17	U	7	0	0	0	0
17	V	11	0	0	0	0
17	W	5	0	0	0	0
17	X	9	0	0	0	0
17	Y	12	0	0	0	0
17	Z	12	0	0	0	0
17	a	9	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	b	4	0	0	1	0
All	All	49433	0	49032	177	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 177 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)
13:a:65:ARG:HG2	13:a:65:ARG:HH21	1.19	1.07
13:M:30:TYR:CD1	13:M:35:ARG:NE	2.31	0.97
13:M:30:TYR:CE1	13:M:35:ARG:NH2	2.42	0.88
14:N:141:ASN:O	14:N:141:ASN:ND2	2.08	0.86
14:b:141:ASN:ND2	14:b:141:ASN:O	2.09	0.84

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%)	241 (97%)	7 (3%)	0	100	100
1	O	248/250 (99%)	241 (97%)	7 (3%)	0	100	100
2	B	242/258 (94%)	236 (98%)	4 (2%)	2 (1%)	16	45
2	P	242/258 (94%)	236 (98%)	4 (2%)	2 (1%)	16	45
3	C	238/254 (94%)	229 (96%)	7 (3%)	2 (1%)	16	45
3	Q	238/254 (94%)	229 (96%)	7 (3%)	2 (1%)	16	45
4	D	231/260 (89%)	226 (98%)	5 (2%)	0	100	100
4	R	231/260 (89%)	226 (98%)	5 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	235 (98%)	6 (2%)	0	100	100
6	T	241/288 (84%)	235 (98%)	6 (2%)	0	100	100
7	G	239/252 (95%)	234 (98%)	5 (2%)	0	100	100
7	U	239/252 (95%)	234 (98%)	5 (2%)	0	100	100
8	H	220/232 (95%)	213 (97%)	7 (3%)	0	100	100
8	V	220/232 (95%)	213 (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%)	190 (98%)	3 (2%)	0	100	100
10	X	193/198 (98%)	190 (98%)	3 (2%)	0	100	100
11	K	210/212 (99%)	204 (97%)	6 (3%)	0	100	100
11	Y	210/212 (99%)	205 (98%)	5 (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%)	219 (95%)	11 (5%)	1 (0%)	30	60
13	a	231/246 (94%)	218 (94%)	12 (5%)	1 (0%)	30	60
14	N	187/215 (87%)	178 (95%)	9 (5%)	0	100	100
14	b	187/215 (87%)	178 (95%)	9 (5%)	0	100	100
All	All	6262/6652 (94%)	6076 (97%)	176 (3%)	10 (0%)	44	73

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	51	VAL
3	C	202	GLN
2	P	51	VAL
3	Q	202	GLN
3	C	205	ALA

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar

resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	209/209 (100%)	205 (98%)	4 (2%)	52	81
1	O	209/209 (100%)	205 (98%)	4 (2%)	52	81
2	B	203/216 (94%)	196 (97%)	7 (3%)	32	67
2	P	203/216 (94%)	196 (97%)	7 (3%)	32	67
3	C	212/226 (94%)	207 (98%)	5 (2%)	44	76
3	Q	212/226 (94%)	207 (98%)	5 (2%)	44	76
4	D	194/215 (90%)	186 (96%)	8 (4%)	26	60
4	R	194/215 (90%)	186 (96%)	8 (4%)	26	60
5	E	190/193 (98%)	185 (97%)	5 (3%)	41	74
5	S	190/193 (98%)	185 (97%)	5 (3%)	41	74
6	F	201/239 (84%)	195 (97%)	6 (3%)	36	71
6	T	201/239 (84%)	195 (97%)	6 (3%)	36	71
7	G	206/210 (98%)	201 (98%)	5 (2%)	44	76
7	U	206/210 (98%)	201 (98%)	5 (2%)	44	76
8	H	181/190 (95%)	177 (98%)	4 (2%)	47	78
8	V	181/190 (95%)	177 (98%)	4 (2%)	47	78
9	I	172/173 (99%)	170 (99%)	2 (1%)	67	89
9	W	172/173 (99%)	170 (99%)	2 (1%)	67	89
10	J	173/175 (99%)	170 (98%)	3 (2%)	56	83
10	X	173/175 (99%)	167 (96%)	6 (4%)	31	66
11	K	169/169 (100%)	164 (97%)	5 (3%)	36	71
11	Y	169/169 (100%)	165 (98%)	4 (2%)	44	76
12	L	185/185 (100%)	179 (97%)	6 (3%)	34	69
12	Z	185/185 (100%)	179 (97%)	6 (3%)	34	69
13	M	199/208 (96%)	194 (98%)	5 (2%)	42	75
13	a	199/208 (96%)	194 (98%)	5 (2%)	42	75
14	N	159/179 (89%)	147 (92%)	12 (8%)	11	33
14	b	159/179 (89%)	148 (93%)	11 (7%)	13	37
All	All	5306/5574 (95%)	5151 (97%)	155 (3%)	37	72

5 of 155 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	U	181	LYS
13	a	104	ARG
8	V	153	LYS
11	Y	116	ASP
14	b	141	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 101 such sidechains are listed below:

Mol	Chain	Res	Type
2	P	232	GLN
5	S	151	ASN
14	b	38	HIS
3	Q	116	GLN
4	R	91	HIS

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 oligosaccharides 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 [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, 95th 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 ²)	Q<0.9
1	A	250/250 (100%)	-0.39	3 (1%) 76 71	38, 54, 96, 150	0
1	O	250/250 (100%)	-0.40	2 (0%) 82 78	45, 62, 109, 155	0
2	B	244/258 (94%)	-0.26	6 (2%) 58 52	40, 62, 113, 170	0
2	P	244/258 (94%)	-0.27	5 (2%) 64 58	44, 64, 110, 164	0
3	C	240/254 (94%)	-0.32	4 (1%) 69 63	41, 65, 130, 165	0
3	Q	240/254 (94%)	0.02	12 (5%) 35 30	51, 82, 166, 194	0
4	D	235/260 (90%)	-0.36	2 (0%) 81 76	45, 67, 102, 141	0
4	R	235/260 (90%)	-0.24	1 (0%) 89 86	52, 73, 115, 169	0
5	E	231/234 (98%)	-0.36	0 100 100	44, 69, 109, 148	0
5	S	231/234 (98%)	-0.13	3 (1%) 74 69	50, 79, 129, 167	0
6	F	243/288 (84%)	-0.46	0 100 100	40, 63, 109, 139	0
6	T	243/288 (84%)	-0.29	1 (0%) 89 86	45, 73, 131, 167	0
7	G	241/252 (95%)	-0.49	0 100 100	38, 56, 94, 141	0
7	U	241/252 (95%)	-0.43	1 (0%) 89 86	35, 61, 97, 142	0
8	H	222/232 (95%)	-0.52	0 100 100	37, 52, 87, 122	0
8	V	222/232 (95%)	-0.55	0 100 100	40, 56, 85, 128	0
9	I	204/205 (99%)	-0.66	0 100 100	34, 51, 78, 101	0
9	W	204/205 (99%)	-0.56	0 100 100	36, 54, 87, 114	0
10	J	195/198 (98%)	-0.52	1 (0%) 87 84	34, 55, 83, 122	0
10	X	195/198 (98%)	-0.48	2 (1%) 79 74	37, 58, 85, 142	0
11	K	212/212 (100%)	-0.33	3 (1%) 73 68	39, 55, 82, 103	0
11	Y	212/212 (100%)	-0.41	1 (0%) 87 84	43, 55, 81, 104	0
12	L	222/222 (100%)	-0.23	13 (5%) 29 25	32, 59, 111, 141	0
12	Z	222/222 (100%)	-0.18	14 (6%) 27 23	36, 58, 111, 148	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	M	233/246 (94%)	-0.46	3 (1%) 74 69	34, 58, 85, 103	0
13	a	233/246 (94%)	-0.43	4 (1%) 69 63	35, 60, 85, 105	0
14	N	191/215 (88%)	-0.39	3 (1%) 70 64	33, 57, 94, 139	0
14	b	191/215 (88%)	-0.33	2 (1%) 79 74	32, 58, 94, 138	0
All	All	6326/6652 (95%)	-0.37	86 (1%) 73 68	32, 61, 111, 194	0

The worst 5 of 86 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	219	ALA	5.0
3	Q	50	LEU	4.8
12	Z	163	GLY	4.5
12	L	166	GLY	4.3
12	L	174	TYR	4.3

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 oligosaccharides 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, 95th 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 ²)	Q<0.9
15	MG	N	201	1/1	0.93	0.18	49,49,49,49	0
15	MG	Z	301	1/1	0.94	0.08	63,63,63,63	0
15	MG	I	301	1/1	0.97	0.04	59,59,59,59	0
15	MG	V	301	1/1	0.98	0.12	68,68,68,68	0
15	MG	Y	301	1/1	0.98	0.10	52,52,52,52	0
15	MG	G	301	1/1	0.98	0.04	49,49,49,49	0
16	CL	N	202	1/1	0.98	0.08	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
16	CL	U	301	1/1	0.98	0.08	56,56,56,56	0
16	CL	b	201	1/1	0.98	0.07	59,59,59,59	0
15	MG	G	302	1/1	0.99	0.14	35,35,35,35	0
15	MG	K	301	1/1	0.99	0.06	43,43,43,43	0
16	CL	G	303	1/1	0.99	0.07	43,43,43,43	0

6.5 Other polymers [i](#)

There are no such residues in this entry.