



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 06:28 PM UTC

PDB ID : 2FHG / pdb_00002fhg
Title : Crystal Structure of Mycobacterial Tuberculosis Proteasome
Authors : Hu, G.; Lin, G.; Wang, M.; Dick, L.; Xu, R.M.; Nathan, C.; Li, H.
Deposited on : 2005-12-23
Resolution : 3.23 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	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
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)	:	2.49

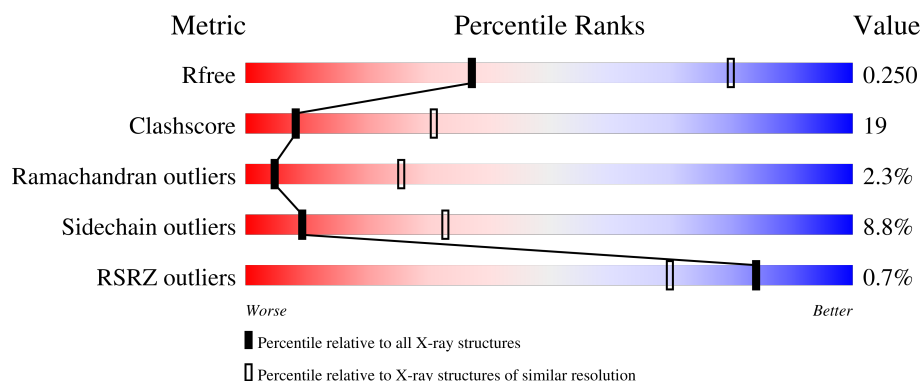
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.23 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}	180053	2153 (3.28-3.20)
Clashscore	190562	2275 (3.28-3.20)
Ramachandran outliers	187476	2233 (3.28-3.20)
Sidechain outliers	187428	2232 (3.28-3.20)
RSRZ outliers	180081	2153 (3.28-3.20)

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	1	250	53%30%5%12%
1	A	250	% 54%30%.12%
1	B	250	53%30%.12%
1	D	250	54%32%.12%
1	F	250	54%30%.12%

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Mol	Chain	Length	Quality of chain
1	I	250	
1	K	250	
1	M	250	
1	O	250	
1	Q	250	
1	S	250	
1	U	250	
1	W	250	
1	Y	250	
2	2	240	
2	C	240	
2	E	240	
2	G	240	
2	H	240	
2	J	240	
2	L	240	
2	N	240	
2	P	240	
2	R	240	
2	T	240	
2	V	240	
2	X	240	
2	Z	240	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 46846 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 20S proteasome, alpha and beta subunits.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	220	Total	C	N	O	S	0	0	0
			1692	1058	309	322	3			
1	B	220	Total	C	N	O	S	0	0	0
			1692	1058	309	322	3			
1	D	220	Total	C	N	O	S	0	0	0
			1692	1058	309	322	3			
1	F	220	Total	C	N	O	S	0	0	0
			1692	1058	309	322	3			
1	I	220	Total	C	N	O	S	0	0	0
			1692	1058	309	322	3			
1	K	220	Total	C	N	O	S	0	0	0
			1692	1058	309	322	3			
1	M	220	Total	C	N	O	S	0	0	0
			1692	1058	309	322	3			
1	O	220	Total	C	N	O	S	0	0	0
			1692	1058	309	322	3			
1	Q	220	Total	C	N	O	S	0	0	0
			1692	1058	309	322	3			
1	S	220	Total	C	N	O	S	0	0	0
			1692	1058	309	322	3			
1	U	220	Total	C	N	O	S	0	0	0
			1692	1058	309	322	3			
1	W	220	Total	C	N	O	S	0	0	0
			1692	1058	309	322	3			
1	Y	220	Total	C	N	O	S	0	0	0
			1692	1058	309	322	3			
1	1	220	Total	C	N	O	S	0	0	0
			1692	1058	309	322	3			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	initiating methionine	GB 13881852

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Chain	Residue	Modelled	Actual	Comment	Reference
A	0	ASN	-	cloning artifact	GB 13881852
A	1	SER	-	cloning artifact	GB 13881852
B	-1	MET	-	initiating methionine	GB 13881852
B	0	ASN	-	cloning artifact	GB 13881852
B	1	SER	-	cloning artifact	GB 13881852
D	-1	MET	-	initiating methionine	GB 13881852
D	0	ASN	-	cloning artifact	GB 13881852
D	1	SER	-	cloning artifact	GB 13881852
F	-1	MET	-	initiating methionine	GB 13881852
F	0	ASN	-	cloning artifact	GB 13881852
F	1	SER	-	cloning artifact	GB 13881852
I	-1	MET	-	initiating methionine	GB 13881852
I	0	ASN	-	cloning artifact	GB 13881852
I	1	SER	-	cloning artifact	GB 13881852
K	-1	MET	-	initiating methionine	GB 13881852
K	0	ASN	-	cloning artifact	GB 13881852
K	1	SER	-	cloning artifact	GB 13881852
M	-1	MET	-	initiating methionine	GB 13881852
M	0	ASN	-	cloning artifact	GB 13881852
M	1	SER	-	cloning artifact	GB 13881852
O	-1	MET	-	initiating methionine	GB 13881852
O	0	ASN	-	cloning artifact	GB 13881852
O	1	SER	-	cloning artifact	GB 13881852
Q	-1	MET	-	initiating methionine	GB 13881852
Q	0	ASN	-	cloning artifact	GB 13881852
Q	1	SER	-	cloning artifact	GB 13881852
S	-1	MET	-	initiating methionine	GB 13881852
S	0	ASN	-	cloning artifact	GB 13881852
S	1	SER	-	cloning artifact	GB 13881852
U	-1	MET	-	initiating methionine	GB 13881852
U	0	ASN	-	cloning artifact	GB 13881852
U	1	SER	-	cloning artifact	GB 13881852
W	-1	MET	-	initiating methionine	GB 13881852
W	0	ASN	-	cloning artifact	GB 13881852
W	1	SER	-	cloning artifact	GB 13881852
Y	-1	MET	-	initiating methionine	GB 13881852
Y	0	ASN	-	cloning artifact	GB 13881852
Y	1	SER	-	cloning artifact	GB 13881852
1	-1	MET	-	initiating methionine	GB 13881852
1	0	ASN	-	cloning artifact	GB 13881852
1	1	SER	-	cloning artifact	GB 13881852

- Molecule 2 is a protein called proteasome, beta subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	222	Total 1638	C 1027	N 282	O 324	S 5	0	0	0
2	C	222	Total 1638	C 1027	N 282	O 324	S 5	0	0	0
2	E	222	Total 1638	C 1027	N 282	O 324	S 5	0	0	0
2	G	222	Total 1638	C 1027	N 282	O 324	S 5	0	0	0
2	J	222	Total 1638	C 1027	N 282	O 324	S 5	0	0	0
2	L	222	Total 1638	C 1027	N 282	O 324	S 5	0	0	0
2	N	222	Total 1638	C 1027	N 282	O 324	S 5	0	0	0
2	P	222	Total 1638	C 1027	N 282	O 324	S 5	0	0	0
2	R	222	Total 1638	C 1027	N 282	O 324	S 5	0	0	0
2	T	222	Total 1638	C 1027	N 282	O 324	S 5	0	0	0
2	V	222	Total 1638	C 1027	N 282	O 324	S 5	0	0	0
2	X	222	Total 1638	C 1027	N 282	O 324	S 5	0	0	0
2	Z	222	Total 1638	C 1027	N 282	O 324	S 5	0	0	0
2	2	222	Total 1638	C 1027	N 282	O 324	S 5	0	0	0

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	535	HIS	-	expression tag	GB 13881852
H	536	HIS	-	expression tag	GB 13881852
H	537	HIS	-	expression tag	GB 13881852
H	538	HIS	-	expression tag	GB 13881852
H	539	HIS	-	expression tag	GB 13881852
H	540	HIS	-	expression tag	GB 13881852
C	535	HIS	-	expression tag	GB 13881852
C	536	HIS	-	expression tag	GB 13881852
C	537	HIS	-	expression tag	GB 13881852
C	538	HIS	-	expression tag	GB 13881852
C	539	HIS	-	expression tag	GB 13881852
C	540	HIS	-	expression tag	GB 13881852

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Chain	Residue	Modelled	Actual	Comment	Reference
E	535	HIS	-	expression tag	GB 13881852
E	536	HIS	-	expression tag	GB 13881852
E	537	HIS	-	expression tag	GB 13881852
E	538	HIS	-	expression tag	GB 13881852
E	539	HIS	-	expression tag	GB 13881852
E	540	HIS	-	expression tag	GB 13881852
G	535	HIS	-	expression tag	GB 13881852
G	536	HIS	-	expression tag	GB 13881852
G	537	HIS	-	expression tag	GB 13881852
G	538	HIS	-	expression tag	GB 13881852
G	539	HIS	-	expression tag	GB 13881852
G	540	HIS	-	expression tag	GB 13881852
J	535	HIS	-	expression tag	GB 13881852
J	536	HIS	-	expression tag	GB 13881852
J	537	HIS	-	expression tag	GB 13881852
J	538	HIS	-	expression tag	GB 13881852
J	539	HIS	-	expression tag	GB 13881852
J	540	HIS	-	expression tag	GB 13881852
L	535	HIS	-	expression tag	GB 13881852
L	536	HIS	-	expression tag	GB 13881852
L	537	HIS	-	expression tag	GB 13881852
L	538	HIS	-	expression tag	GB 13881852
L	539	HIS	-	expression tag	GB 13881852
L	540	HIS	-	expression tag	GB 13881852
N	535	HIS	-	expression tag	GB 13881852
N	536	HIS	-	expression tag	GB 13881852
N	537	HIS	-	expression tag	GB 13881852
N	538	HIS	-	expression tag	GB 13881852
N	539	HIS	-	expression tag	GB 13881852
N	540	HIS	-	expression tag	GB 13881852
P	535	HIS	-	expression tag	GB 13881852
P	536	HIS	-	expression tag	GB 13881852
P	537	HIS	-	expression tag	GB 13881852
P	538	HIS	-	expression tag	GB 13881852
P	539	HIS	-	expression tag	GB 13881852
P	540	HIS	-	expression tag	GB 13881852
R	535	HIS	-	expression tag	GB 13881852
R	536	HIS	-	expression tag	GB 13881852
R	537	HIS	-	expression tag	GB 13881852
R	538	HIS	-	expression tag	GB 13881852
R	539	HIS	-	expression tag	GB 13881852
R	540	HIS	-	expression tag	GB 13881852

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Chain	Residue	Modelled	Actual	Comment	Reference
T	535	HIS	-	expression tag	GB 13881852
T	536	HIS	-	expression tag	GB 13881852
T	537	HIS	-	expression tag	GB 13881852
T	538	HIS	-	expression tag	GB 13881852
T	539	HIS	-	expression tag	GB 13881852
T	540	HIS	-	expression tag	GB 13881852
V	535	HIS	-	expression tag	GB 13881852
V	536	HIS	-	expression tag	GB 13881852
V	537	HIS	-	expression tag	GB 13881852
V	538	HIS	-	expression tag	GB 13881852
V	539	HIS	-	expression tag	GB 13881852
V	540	HIS	-	expression tag	GB 13881852
X	535	HIS	-	expression tag	GB 13881852
X	536	HIS	-	expression tag	GB 13881852
X	537	HIS	-	expression tag	GB 13881852
X	538	HIS	-	expression tag	GB 13881852
X	539	HIS	-	expression tag	GB 13881852
X	540	HIS	-	expression tag	GB 13881852
Z	535	HIS	-	expression tag	GB 13881852
Z	536	HIS	-	expression tag	GB 13881852
Z	537	HIS	-	expression tag	GB 13881852
Z	538	HIS	-	expression tag	GB 13881852
Z	539	HIS	-	expression tag	GB 13881852
Z	540	HIS	-	expression tag	GB 13881852
2	535	HIS	-	expression tag	GB 13881852
2	536	HIS	-	expression tag	GB 13881852
2	537	HIS	-	expression tag	GB 13881852
2	538	HIS	-	expression tag	GB 13881852
2	539	HIS	-	expression tag	GB 13881852
2	540	HIS	-	expression tag	GB 13881852

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	2	Total O 2 2	0	0
3	H	1	Total O 1 1	0	0
3	B	7	Total O 7 7	0	0
3	C	6	Total O 6 6	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	11	Total 11	O 11	0	0
3	E	9	Total 9	O 9	0	0
3	F	10	Total 10	O 10	0	0
3	G	9	Total 9	O 9	0	0
3	I	7	Total 7	O 7	0	0
3	J	5	Total 5	O 5	0	0
3	K	15	Total 15	O 15	0	0
3	L	4	Total 4	O 4	0	0
3	M	11	Total 11	O 11	0	0
3	N	7	Total 7	O 7	0	0
3	O	8	Total 8	O 8	0	0
3	P	4	Total 4	O 4	0	0
3	Q	6	Total 6	O 6	0	0
3	R	5	Total 5	O 5	0	0
3	S	13	Total 13	O 13	0	0
3	T	6	Total 6	O 6	0	0
3	U	7	Total 7	O 7	0	0
3	V	10	Total 10	O 10	0	0
3	W	8	Total 8	O 8	0	0
3	X	4	Total 4	O 4	0	0
3	Y	12	Total 12	O 12	0	0

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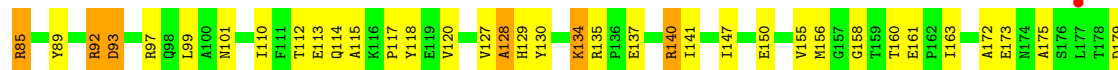
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	Z	7	Total 7	O 7	0	0
3	1	13	Total 13	O 13	0	0
3	2	19	Total 19	O 19	0	0



- Molecule 1: 20S proteasome, alpha and beta subunits

Chain F: 54% 30% 12%



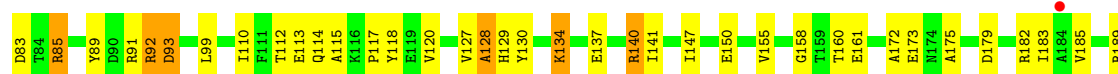
- Molecule 1: 20S proteasome, alpha and beta subunits

Chain I: 53% 31% 12%



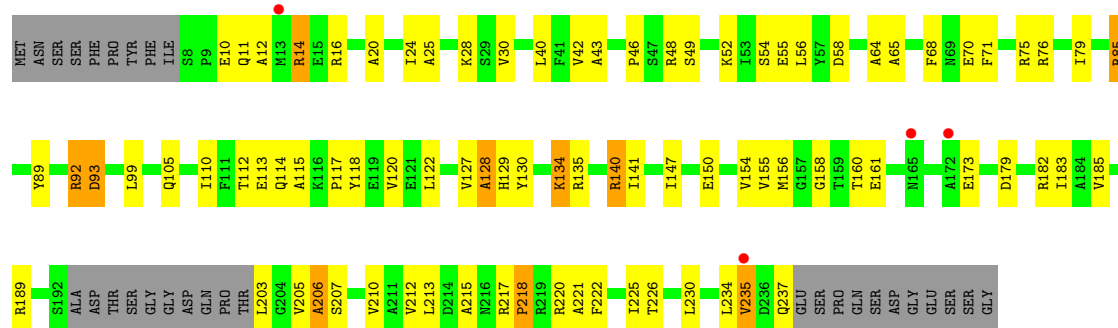
- Molecule 1: 20S proteasome, alpha and beta subunits

Chain K: 53% 32% 12%

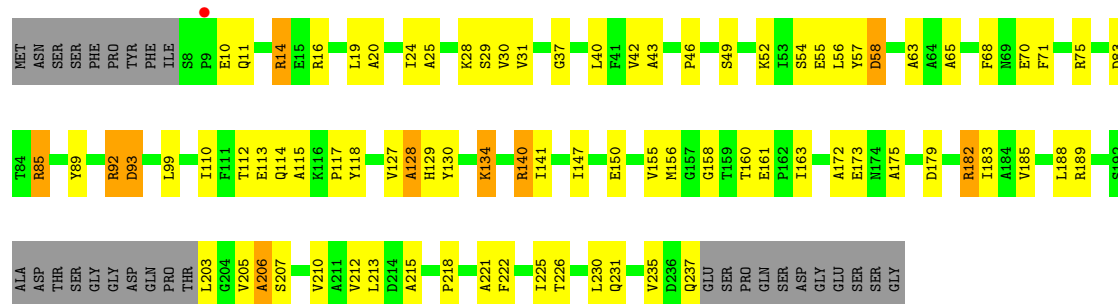


- Molecule 1: 20S proteasome, alpha and beta subunits

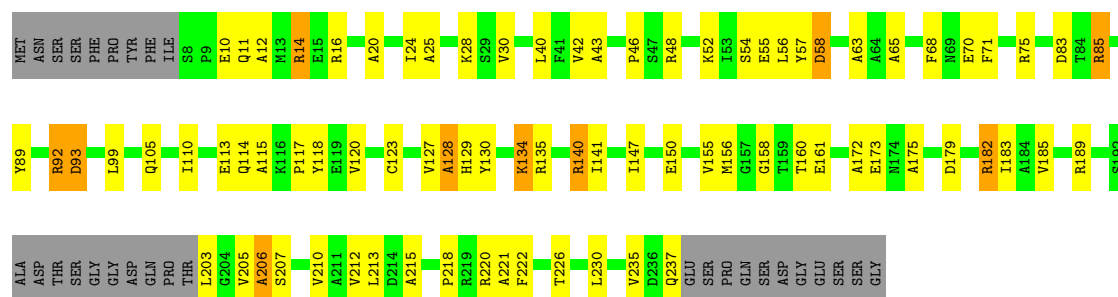
Chain M: 54% 30% 12%



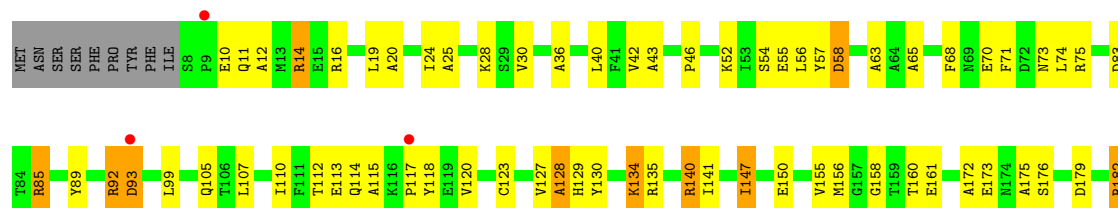
- Molecule 1: 20S proteasome, alpha and beta subunits



- Molecule 1: 20S proteasome, alpha and beta subunits

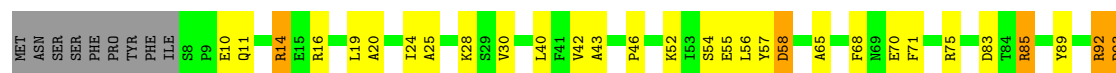


- Molecule 1: 20S proteasome, alpha and beta subunits





- Molecule 1: 20S proteasome, alpha and beta subunits



- Molecule 1: 20S proteasome, alpha and beta subunits

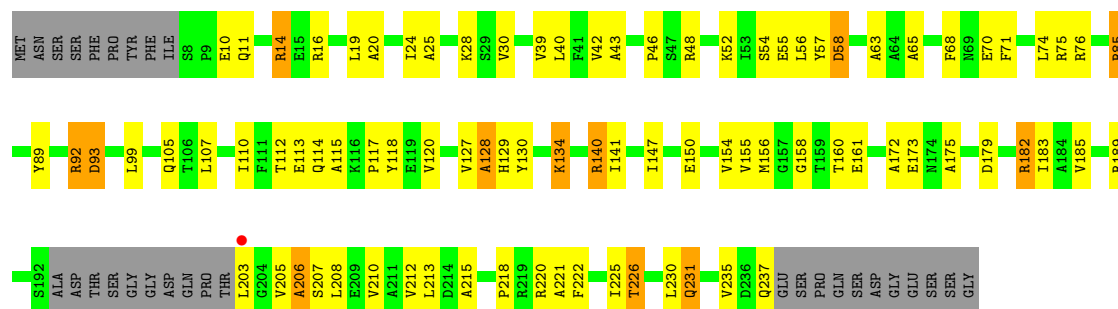


- Molecule 1: 20S proteasome, alpha and beta subunits

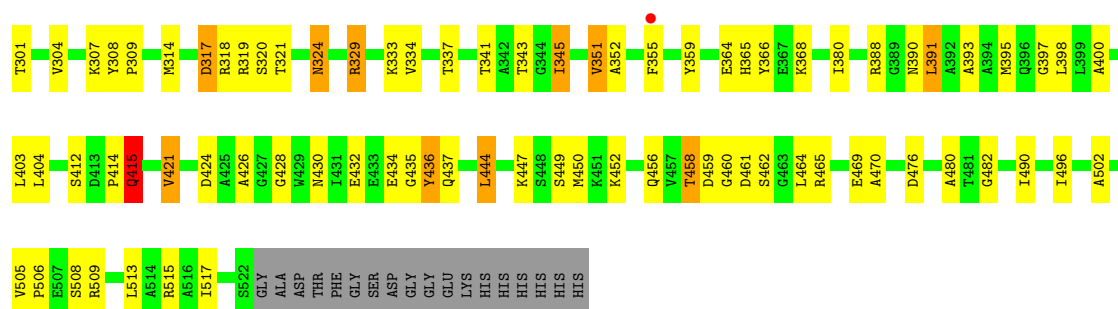


- Molecule 1: 20S proteasome, alpha and beta subunits

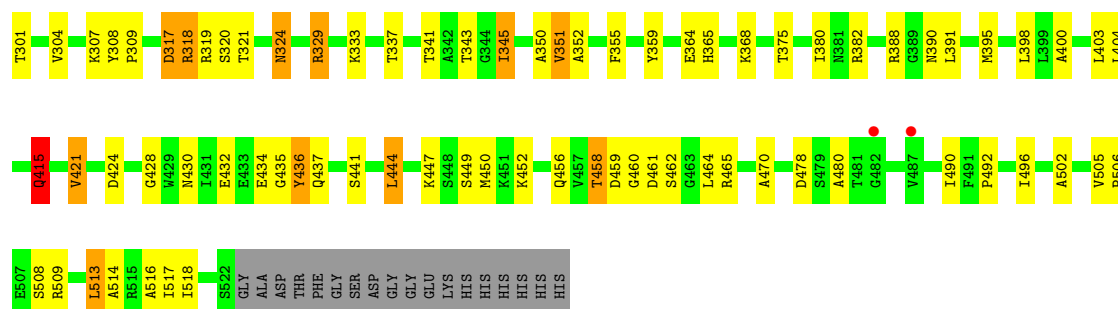




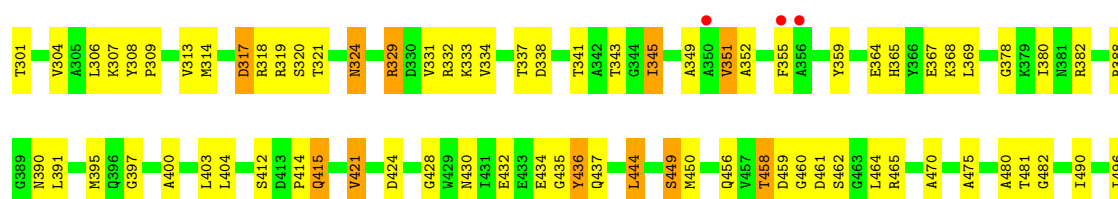
- Molecule 2: proteasome, beta subunit

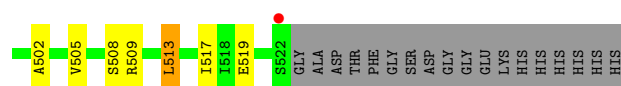


- Molecule 2: proteasome, beta subunit

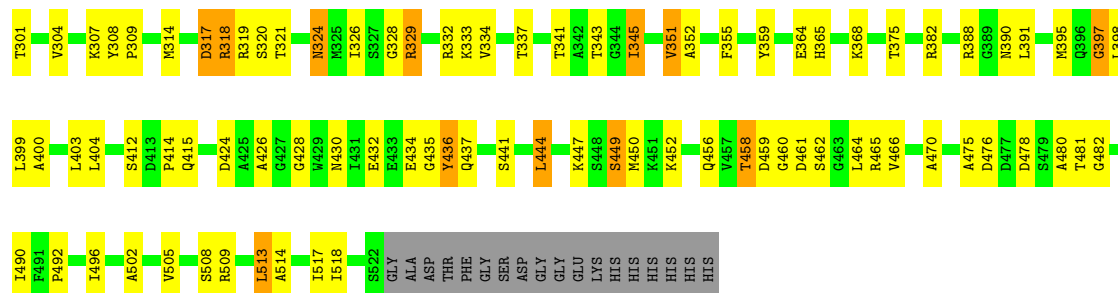


- Molecule 2: proteasome, beta subunit

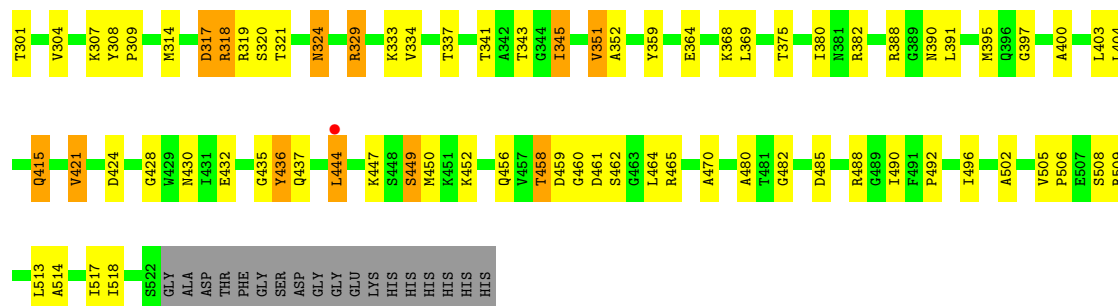




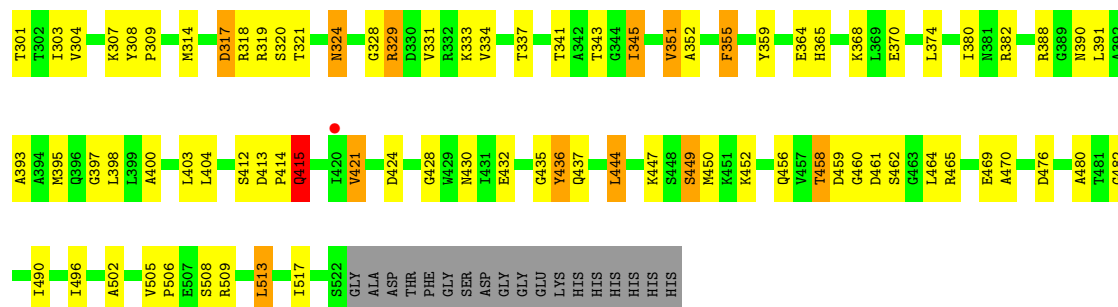
- Molecule 2: proteasome, beta subunit



- Molecule 2: proteasome, beta subunit

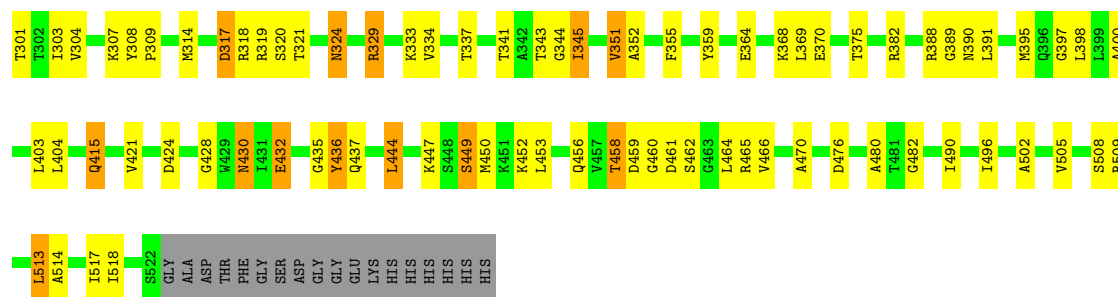


- Molecule 2: proteasome, beta subunit

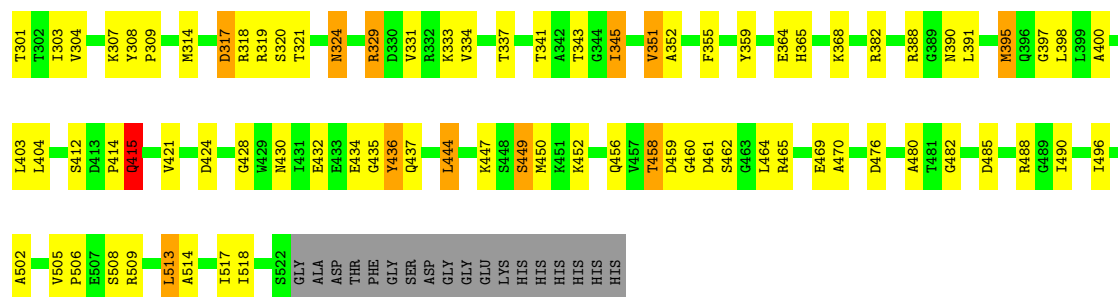


- Molecule 2: proteasome, beta subunit

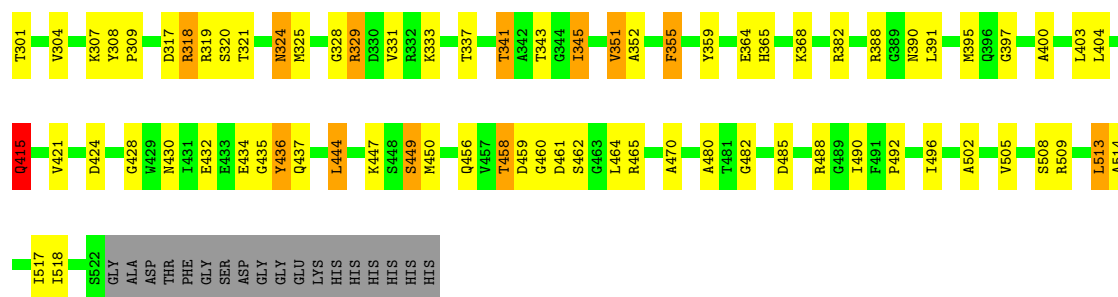




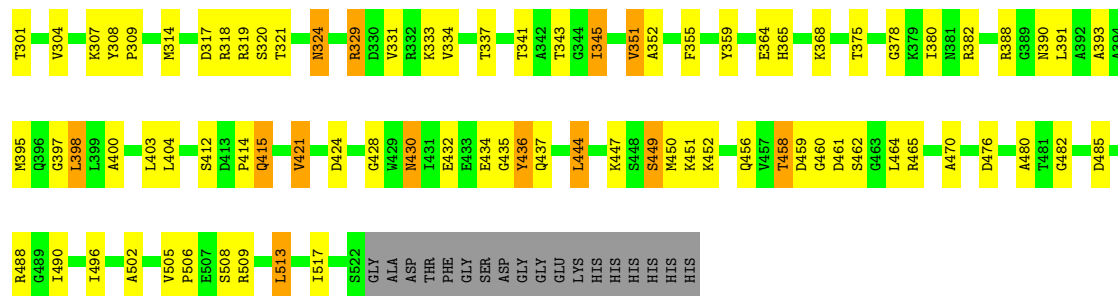
- Molecule 2: proteasome, beta subunit



- Molecule 2: proteasome, beta subunit

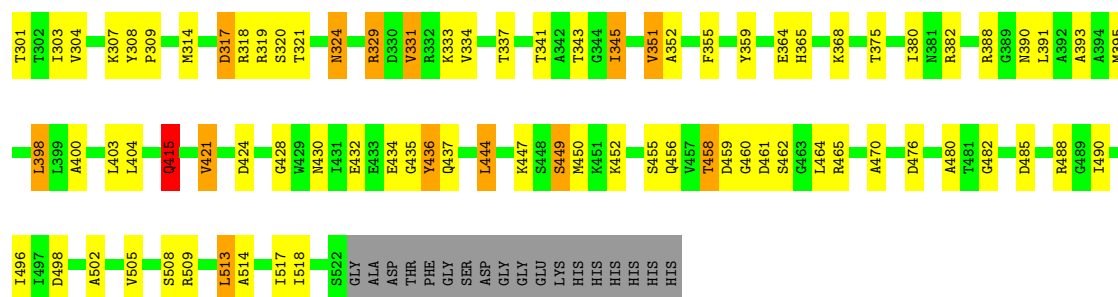


- Molecule 2: proteasome, beta subunit



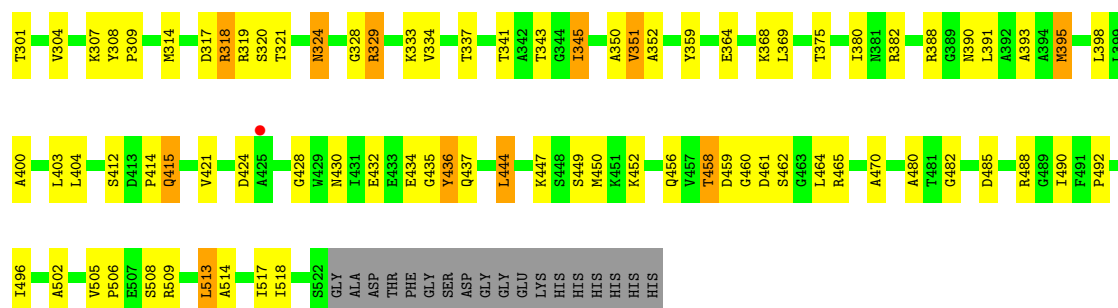
- Molecule 2: proteasome, beta subunit

Chain V: 



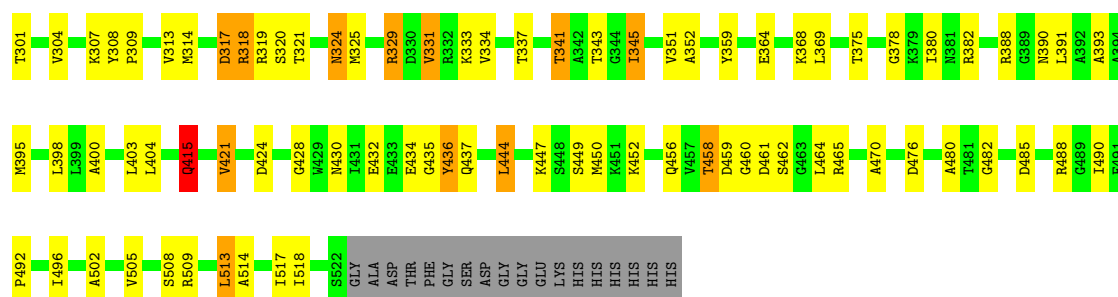
• Molecule 2: proteasome, beta subunit

Chain X: 



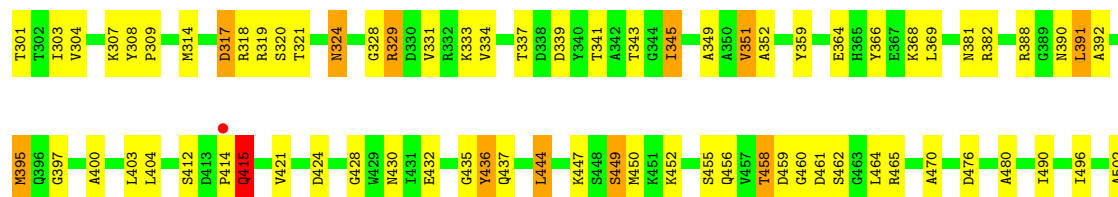
• Molecule 2: proteasome, beta subunit

Chain Z: 



• Molecule 2: proteasome, beta subunit

Chain 2: 



V505	P506	S507	S508	R509	L513	I517	S522	GLY	ALA	ASP	THR	PHE	GLY	SER	ASP	GLY	GLY	GLU	LYS	HIS	HIS	HIS	HIS	HIS	HIS
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4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	173.33Å 113.80Å 200.13Å 90.00° 113.93° 90.00°	Depositor
Resolution (Å)	50.00 – 3.23 50.00 – 3.23	Depositor EDS
% Data completeness (in resolution range)	79.6 (50.00-3.23) 79.8 (50.00-3.23)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.49 (at 3.25Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.243 , 0.266 0.247 , 0.250	Depositor DCC
R_{free} test set	2776 reflections (3.04%)	wwPDB-VP
Wilson B-factor (Å ²)	82.0	Xtriage
Anisotropy	0.332	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 105.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.046 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	46846	wwPDB-VP
Average B, all atoms (Å ²)	99.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.55% 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

5.1 Standard geometry

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	1	0.56	0/1717	0.89	0/2320
1	A	0.68	1/1717 (0.1%)	0.92	0/2320
1	B	0.62	0/1717	0.91	0/2320
1	D	0.61	0/1717	0.90	0/2320
1	F	0.59	0/1717	0.89	0/2320
1	I	0.58	0/1717	0.88	0/2320
1	K	0.57	0/1717	0.90	0/2320
1	M	0.59	1/1717 (0.1%)	0.89	0/2320
1	O	0.58	0/1717	0.90	0/2320
1	Q	0.59	0/1717	0.90	0/2320
1	S	0.57	0/1717	0.88	0/2320
1	U	0.57	0/1717	0.90	0/2320
1	W	0.61	0/1717	0.89	0/2320
1	Y	0.57	0/1717	0.88	0/2320
2	2	0.57	0/1662	0.91	1/2254 (0.0%)
2	C	0.69	0/1662	0.92	1/2254 (0.0%)
2	E	0.69	0/1662	0.94	1/2254 (0.0%)
2	G	0.63	0/1662	0.93	0/2254
2	H	0.71	0/1662	0.94	1/2254 (0.0%)
2	J	0.64	0/1662	0.91	1/2254 (0.0%)
2	L	0.66	0/1662	0.93	1/2254 (0.0%)
2	N	0.64	0/1662	0.95	2/2254 (0.1%)
2	P	0.65	0/1662	0.91	1/2254 (0.0%)
2	R	0.65	0/1662	0.94	1/2254 (0.0%)
2	T	0.63	0/1662	0.91	1/2254 (0.0%)
2	V	0.63	0/1662	0.93	1/2254 (0.0%)
2	X	0.66	0/1662	0.91	1/2254 (0.0%)
2	Z	0.64	0/1662	0.92	1/2254 (0.0%)
All	All	0.62	2/47306 (0.0%)	0.91	14/64036 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	235	VAL	CA-CB	5.09	1.60	1.54
1	M	235	VAL	CA-CB	5.02	1.60	1.54

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	415	GLN	N-CA-C	-6.64	104.33	114.16
2	2	415	GLN	N-CA-C	-6.63	103.81	114.09
2	Z	415	GLN	N-CA-C	-6.58	104.42	114.16
2	E	415	GLN	N-CA-C	-6.46	104.61	114.16
2	V	415	GLN	N-CA-C	-6.31	104.83	114.16

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	1	1692	0	1688	77	0
1	A	1692	0	1688	77	4
1	B	1692	0	1688	76	0
1	D	1692	0	1688	72	4
1	F	1692	0	1688	80	0
1	I	1692	0	1688	75	2
1	K	1692	0	1688	84	0
1	M	1692	0	1688	89	0
1	O	1692	0	1688	78	0
1	Q	1692	0	1688	71	0
1	S	1692	0	1688	80	0
1	U	1692	0	1688	69	2
1	W	1692	0	1688	77	1
1	Y	1692	0	1688	73	0
2	2	1638	0	1630	70	1
2	C	1638	0	1630	61	0
2	E	1638	0	1630	64	1
2	G	1638	0	1630	71	3
2	H	1638	0	1630	64	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	J	1638	0	1630	59	2
2	L	1638	0	1630	71	0
2	N	1638	0	1630	68	1
2	P	1638	0	1630	66	1
2	R	1638	0	1630	58	0
2	T	1638	0	1630	65	0
2	V	1638	0	1630	68	2
2	X	1638	0	1630	63	3
2	Z	1638	0	1630	65	1
3	1	13	0	0	10	0
3	2	19	0	0	8	0
3	A	2	0	0	2	0
3	B	7	0	0	2	0
3	C	6	0	0	0	0
3	D	11	0	0	3	0
3	E	9	0	0	3	0
3	F	10	0	0	1	0
3	G	9	0	0	3	0
3	H	1	0	0	3	0
3	I	7	0	0	3	0
3	J	5	0	0	0	0
3	K	15	0	0	8	0
3	L	4	0	0	3	0
3	M	11	0	0	5	0
3	N	7	0	0	5	0
3	O	8	0	0	8	0
3	P	4	0	0	0	0
3	Q	6	0	0	2	0
3	R	5	0	0	2	0
3	S	13	0	0	3	0
3	T	6	0	0	4	0
3	U	7	0	0	1	0
3	V	10	0	0	4	0
3	W	8	0	0	3	0
3	X	4	0	0	1	0
3	Y	12	0	0	8	0
3	Z	7	0	0	4	0
All	All	46846	0	46452	1798	14

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 19.

The worst 5 of 1798 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)
2:J:444:LEU:HD12	2:Z:444:LEU:HD12	1.27	1.15
2:P:304:VAL:HG21	2:P:450:MET:HE1	1.30	1.13
2:L:444:LEU:HD12	2:P:444:LEU:HD12	1.30	1.13
2:J:452:LYS:HG3	3:Z:190:HOH:O	1.47	1.12
2:H:304:VAL:HG21	2:H:450:MET:HE1	1.32	1.07

The worst 5 of 14 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:465:ARG:NE	2:X:458:THR:CG2[2_554]	1.40	0.80
1:A:236:ASP:O	1:D:133:THR:OG1[2_655]	1.59	0.61
2:N:456:GLN:NE2	2:Z:415:GLN:OE1[1_565]	1.83	0.37
1:W:228:SER:O	2:2:414:PRO:CB[2_544]	1.97	0.23
2:J:456:GLN:NE2	2:V:415:GLN:OE1[1_545]	2.00	0.20

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	1	216/250 (86%)	188 (87%)	22 (10%)	6 (3%)	4	22
1	A	216/250 (86%)	192 (89%)	19 (9%)	5 (2%)	5	25
1	B	216/250 (86%)	189 (88%)	21 (10%)	6 (3%)	4	22
1	D	216/250 (86%)	193 (89%)	18 (8%)	5 (2%)	5	25
1	F	216/250 (86%)	190 (88%)	20 (9%)	6 (3%)	4	22
1	I	216/250 (86%)	189 (88%)	22 (10%)	5 (2%)	5	25
1	K	216/250 (86%)	191 (88%)	20 (9%)	5 (2%)	5	25
1	M	216/250 (86%)	187 (87%)	24 (11%)	5 (2%)	5	25
1	O	216/250 (86%)	188 (87%)	23 (11%)	5 (2%)	5	25
1	Q	216/250 (86%)	188 (87%)	23 (11%)	5 (2%)	5	25

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	S	216/250 (86%)	189 (88%)	22 (10%)	5 (2%)	5	25
1	U	216/250 (86%)	189 (88%)	22 (10%)	5 (2%)	5	25
1	W	216/250 (86%)	192 (89%)	19 (9%)	5 (2%)	5	25
1	Y	216/250 (86%)	187 (87%)	23 (11%)	6 (3%)	4	22
2	2	220/240 (92%)	195 (89%)	22 (10%)	3 (1%)	9	35
2	C	220/240 (92%)	195 (89%)	22 (10%)	3 (1%)	9	35
2	E	220/240 (92%)	196 (89%)	19 (9%)	5 (2%)	5	25
2	G	220/240 (92%)	196 (89%)	18 (8%)	6 (3%)	4	22
2	H	220/240 (92%)	193 (88%)	22 (10%)	5 (2%)	5	25
2	J	220/240 (92%)	194 (88%)	22 (10%)	4 (2%)	6	31
2	L	220/240 (92%)	194 (88%)	21 (10%)	5 (2%)	5	25
2	N	220/240 (92%)	198 (90%)	16 (7%)	6 (3%)	4	22
2	P	220/240 (92%)	195 (89%)	19 (9%)	6 (3%)	4	22
2	R	220/240 (92%)	193 (88%)	22 (10%)	5 (2%)	5	25
2	T	220/240 (92%)	195 (89%)	19 (9%)	6 (3%)	4	22
2	V	220/240 (92%)	194 (88%)	21 (10%)	5 (2%)	5	25
2	X	220/240 (92%)	193 (88%)	23 (10%)	4 (2%)	6	31
2	Z	220/240 (92%)	192 (87%)	24 (11%)	4 (2%)	6	31
All	All	6104/6860 (89%)	5375 (88%)	588 (10%)	141 (2%)	5	25

5 of 141 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	128	ALA
1	B	128	ALA
1	D	128	ALA
1	F	128	ALA
1	I	128	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	1	169/194 (87%)	155 (92%)	14 (8%)	10	36
1	A	169/194 (87%)	157 (93%)	12 (7%)	13	42
1	B	169/194 (87%)	156 (92%)	13 (8%)	12	39
1	D	169/194 (87%)	156 (92%)	13 (8%)	12	39
1	F	169/194 (87%)	156 (92%)	13 (8%)	12	39
1	I	169/194 (87%)	157 (93%)	12 (7%)	13	42
1	K	169/194 (87%)	157 (93%)	12 (7%)	13	42
1	M	169/194 (87%)	157 (93%)	12 (7%)	13	42
1	O	169/194 (87%)	155 (92%)	14 (8%)	10	36
1	Q	169/194 (87%)	157 (93%)	12 (7%)	13	42
1	S	169/194 (87%)	156 (92%)	13 (8%)	12	39
1	U	169/194 (87%)	156 (92%)	13 (8%)	12	39
1	W	169/194 (87%)	158 (94%)	11 (6%)	15	45
1	Y	169/194 (87%)	158 (94%)	11 (6%)	15	45
2	2	165/178 (93%)	149 (90%)	16 (10%)	8	30
2	C	165/178 (93%)	148 (90%)	17 (10%)	7	27
2	E	165/178 (93%)	147 (89%)	18 (11%)	6	25
2	G	165/178 (93%)	150 (91%)	15 (9%)	9	31
2	H	165/178 (93%)	149 (90%)	16 (10%)	8	30
2	J	165/178 (93%)	150 (91%)	15 (9%)	9	31
2	L	165/178 (93%)	148 (90%)	17 (10%)	7	27
2	N	165/178 (93%)	148 (90%)	17 (10%)	7	27
2	P	165/178 (93%)	147 (89%)	18 (11%)	6	25
2	R	165/178 (93%)	146 (88%)	19 (12%)	5	23
2	T	165/178 (93%)	148 (90%)	17 (10%)	7	27
2	V	165/178 (93%)	148 (90%)	17 (10%)	7	27
2	X	165/178 (93%)	149 (90%)	16 (10%)	8	30
2	Z	165/178 (93%)	148 (90%)	17 (10%)	7	27
All	All	4676/5208 (90%)	4266 (91%)	410 (9%)	9	33

5 of 410 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	P	458	THR
2	T	415	GLN
2	2	391	LEU
1	Q	113	GLU
2	R	444	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 150 such sidechains are listed below:

Mol	Chain	Res	Type
1	U	165	ASN
1	1	105	GLN
2	V	415	GLN
2	X	456	GLN
1	I	129	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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	1	220/250 (88%)	0.03	1 (0%) 87 76	100, 100, 100, 100	0
1	A	220/250 (88%)	0.04	3 (1%) 73 54	100, 100, 100, 100	0
1	B	220/250 (88%)	-0.01	1 (0%) 87 76	100, 100, 100, 100	0
1	D	220/250 (88%)	0.05	1 (0%) 87 76	100, 100, 100, 100	0
1	F	220/250 (88%)	0.09	1 (0%) 87 76	100, 100, 100, 100	0
1	I	220/250 (88%)	0.14	2 (0%) 81 64	100, 100, 100, 100	0
1	K	220/250 (88%)	0.33	5 (2%) 61 41	100, 100, 100, 100	0
1	M	220/250 (88%)	0.16	4 (1%) 67 48	100, 100, 100, 100	0
1	O	220/250 (88%)	0.01	1 (0%) 87 76	100, 100, 100, 100	0
1	Q	220/250 (88%)	-0.01	0 100 100	100, 100, 100, 100	0
1	S	220/250 (88%)	0.26	6 (2%) 56 37	100, 100, 100, 100	0
1	U	220/250 (88%)	-0.10	0 100 100	100, 100, 100, 100	0
1	W	220/250 (88%)	0.08	4 (1%) 67 48	100, 100, 100, 100	0
1	Y	220/250 (88%)	0.37	6 (2%) 56 37	100, 100, 100, 100	0
2	2	222/240 (92%)	0.08	1 (0%) 87 76	100, 100, 100, 100	0
2	C	222/240 (92%)	0.02	2 (0%) 81 64	100, 100, 100, 100	0
2	E	222/240 (92%)	0.12	4 (1%) 67 48	100, 100, 100, 100	0
2	G	222/240 (92%)	0.04	0 100 100	100, 100, 100, 100	0
2	H	222/240 (92%)	0.07	1 (0%) 87 76	100, 100, 100, 100	0
2	J	222/240 (92%)	-0.05	1 (0%) 87 76	100, 100, 100, 100	0
2	L	222/240 (92%)	0.10	1 (0%) 87 76	100, 100, 100, 100	0
2	N	222/240 (92%)	-0.10	0 100 100	100, 100, 100, 100	0
2	P	222/240 (92%)	-0.10	0 100 100	100, 100, 100, 100	0
2	R	222/240 (92%)	-0.03	0 100 100	100, 100, 100, 100	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
2	T	222/240 (92%)	-0.00	0 100 100	100, 100, 100, 100	0
2	V	222/240 (92%)	-0.12	0 100 100	100, 100, 100, 100	0
2	X	222/240 (92%)	-0.07	1 (0%) 87 76	100, 100, 100, 100	0
2	Z	222/240 (92%)	-0.06	0 100 100	100, 100, 100, 100	0
All	All	6188/6860 (90%)	0.05	46 (0%) 84 70	100, 100, 100, 100	0

The worst 5 of 46 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	235	VAL	5.3
1	M	235	VAL	3.8
1	A	177	LEU	3.5
2	2	414	PRO	3.4
2	E	350	ALA	3.3

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.