



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 10:09 AM GMT

PDB ID : 3KRD  
Title : Crystal Structure of Mycobacterium Tuberculosis Proteasome in complex with  
Fellutamide B  
Authors : Li, D.; Li, H.  
Deposited on : 2009-11-18  
Resolution : 2.50 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  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
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) : trunk26865

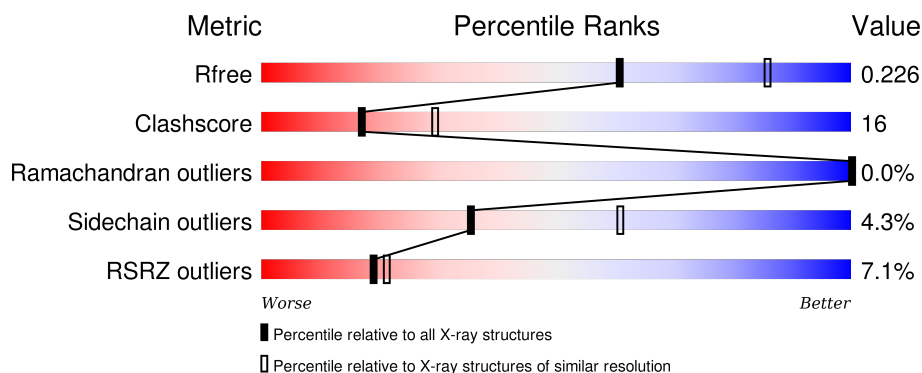
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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))
$R_{free}$	91344	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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	1	248	<div> <div>10%</div> <div> <div>52%</div> <div>31%</div> <div>•</div> <div>13%</div> </div> </div>
1	A	248	<div> <div>14%</div> <div> <div>54%</div> <div>31%</div> <div>•</div> <div>14%</div> </div> </div>
1	B	248	<div> <div>7%</div> <div> <div>58%</div> <div>27%</div> <div>•</div> <div>14%</div> </div> </div>
1	D	248	<div> <div>20%</div> <div> <div>45%</div> <div>37%</div> <div>•</div> <div>14%</div> </div> </div>
1	F	248	<div> <div>6%</div> <div> <div>54%</div> <div>31%</div> <div>•</div> <div>13%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	I	248	
1	K	248	
1	M	248	
1	O	248	
1	Q	248	
1	S	248	
1	U	248	
1	W	248	
1	Y	248	
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	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	FEB	Z	300	-	-	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 48828 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	214	Total	C	N	O	S	0	0	0
			1650	1033	302	312	3			
1	B	213	Total	C	N	O	S	0	0	0
			1642	1027	301	311	3			
1	D	213	Total	C	N	O	S	0	0	0
			1646	1031	301	311	3			
1	F	216	Total	C	N	O	S	0	0	0
			1661	1040	304	314	3			
1	I	215	Total	C	N	O	S	0	0	0
			1654	1035	303	313	3			
1	K	215	Total	C	N	O	S	0	0	0
			1654	1035	303	313	3			
1	M	214	Total	C	N	O	S	0	0	0
			1650	1033	302	312	3			
1	O	214	Total	C	N	O	S	0	0	0
			1650	1033	302	312	3			
1	Q	214	Total	C	N	O	S	0	0	0
			1650	1033	302	312	3			
1	S	215	Total	C	N	O	S	0	0	0
			1657	1038	303	313	3			
1	U	214	Total	C	N	O	S	0	0	0
			1650	1033	302	312	3			
1	W	215	Total	C	N	O	S	0	0	0
			1654	1035	303	313	3			
1	Y	216	Total	C	N	O	S	0	0	0
			1661	1040	304	314	3			
1	1	215	Total	C	N	O	S	0	0	0
			1654	1035	303	313	3			

- Molecule 2 is a protein called Proteasome subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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	H	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	229	Total 1683	C 1054	N 289	O 335	S 5	0	0	0
2	T	222	Total 1638	C 1027	N 282	O 324	S 5	0	0	0
2	V	229	Total 1683	C 1054	N 289	O 335	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
C	535	HIS	-	EXPRESSION TAG	UNP O33245
C	536	HIS	-	EXPRESSION TAG	UNP O33245
C	537	HIS	-	EXPRESSION TAG	UNP O33245
C	538	HIS	-	EXPRESSION TAG	UNP O33245
C	539	HIS	-	EXPRESSION TAG	UNP O33245
C	540	HIS	-	EXPRESSION TAG	UNP O33245
E	535	HIS	-	EXPRESSION TAG	UNP O33245
E	536	HIS	-	EXPRESSION TAG	UNP O33245
E	537	HIS	-	EXPRESSION TAG	UNP O33245
E	538	HIS	-	EXPRESSION TAG	UNP O33245
E	539	HIS	-	EXPRESSION TAG	UNP O33245
E	540	HIS	-	EXPRESSION TAG	UNP O33245

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Chain	Residue	Modelled	Actual	Comment	Reference
G	535	HIS	-	EXPRESSION TAG	UNP O33245
G	536	HIS	-	EXPRESSION TAG	UNP O33245
G	537	HIS	-	EXPRESSION TAG	UNP O33245
G	538	HIS	-	EXPRESSION TAG	UNP O33245
G	539	HIS	-	EXPRESSION TAG	UNP O33245
G	540	HIS	-	EXPRESSION TAG	UNP O33245
H	535	HIS	-	EXPRESSION TAG	UNP O33245
H	536	HIS	-	EXPRESSION TAG	UNP O33245
H	537	HIS	-	EXPRESSION TAG	UNP O33245
H	538	HIS	-	EXPRESSION TAG	UNP O33245
H	539	HIS	-	EXPRESSION TAG	UNP O33245
H	540	HIS	-	EXPRESSION TAG	UNP O33245
J	535	HIS	-	EXPRESSION TAG	UNP O33245
J	536	HIS	-	EXPRESSION TAG	UNP O33245
J	537	HIS	-	EXPRESSION TAG	UNP O33245
J	538	HIS	-	EXPRESSION TAG	UNP O33245
J	539	HIS	-	EXPRESSION TAG	UNP O33245
J	540	HIS	-	EXPRESSION TAG	UNP O33245
L	535	HIS	-	EXPRESSION TAG	UNP O33245
L	536	HIS	-	EXPRESSION TAG	UNP O33245
L	537	HIS	-	EXPRESSION TAG	UNP O33245
L	538	HIS	-	EXPRESSION TAG	UNP O33245
L	539	HIS	-	EXPRESSION TAG	UNP O33245
L	540	HIS	-	EXPRESSION TAG	UNP O33245
N	535	HIS	-	EXPRESSION TAG	UNP O33245
N	536	HIS	-	EXPRESSION TAG	UNP O33245
N	537	HIS	-	EXPRESSION TAG	UNP O33245
N	538	HIS	-	EXPRESSION TAG	UNP O33245
N	539	HIS	-	EXPRESSION TAG	UNP O33245
N	540	HIS	-	EXPRESSION TAG	UNP O33245
P	535	HIS	-	EXPRESSION TAG	UNP O33245
P	536	HIS	-	EXPRESSION TAG	UNP O33245
P	537	HIS	-	EXPRESSION TAG	UNP O33245
P	538	HIS	-	EXPRESSION TAG	UNP O33245
P	539	HIS	-	EXPRESSION TAG	UNP O33245
P	540	HIS	-	EXPRESSION TAG	UNP O33245
R	535	HIS	-	EXPRESSION TAG	UNP O33245
R	536	HIS	-	EXPRESSION TAG	UNP O33245
R	537	HIS	-	EXPRESSION TAG	UNP O33245
R	538	HIS	-	EXPRESSION TAG	UNP O33245
R	539	HIS	-	EXPRESSION TAG	UNP O33245
R	540	HIS	-	EXPRESSION TAG	UNP O33245

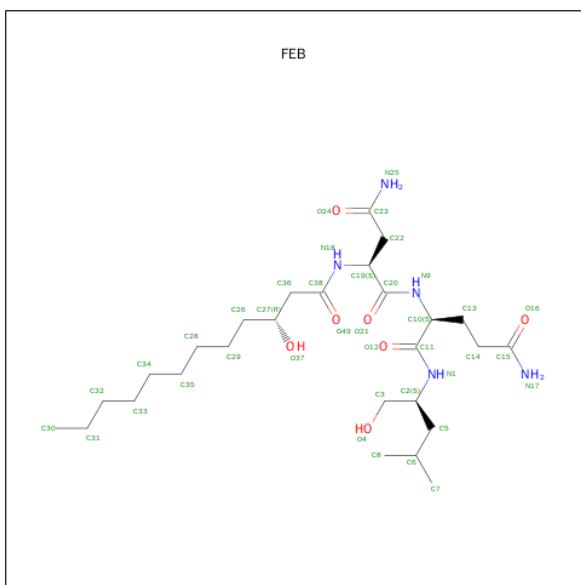
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Chain	Residue	Modelled	Actual	Comment	Reference
T	535	HIS	-	EXPRESSION TAG	UNP O33245
T	536	HIS	-	EXPRESSION TAG	UNP O33245
T	537	HIS	-	EXPRESSION TAG	UNP O33245
T	538	HIS	-	EXPRESSION TAG	UNP O33245
T	539	HIS	-	EXPRESSION TAG	UNP O33245
T	540	HIS	-	EXPRESSION TAG	UNP O33245
V	535	HIS	-	EXPRESSION TAG	UNP O33245
V	536	HIS	-	EXPRESSION TAG	UNP O33245
V	537	HIS	-	EXPRESSION TAG	UNP O33245
V	538	HIS	-	EXPRESSION TAG	UNP O33245
V	539	HIS	-	EXPRESSION TAG	UNP O33245
V	540	HIS	-	EXPRESSION TAG	UNP O33245
X	535	HIS	-	EXPRESSION TAG	UNP O33245
X	536	HIS	-	EXPRESSION TAG	UNP O33245
X	537	HIS	-	EXPRESSION TAG	UNP O33245
X	538	HIS	-	EXPRESSION TAG	UNP O33245
X	539	HIS	-	EXPRESSION TAG	UNP O33245
X	540	HIS	-	EXPRESSION TAG	UNP O33245
Z	535	HIS	-	EXPRESSION TAG	UNP O33245
Z	536	HIS	-	EXPRESSION TAG	UNP O33245
Z	537	HIS	-	EXPRESSION TAG	UNP O33245
Z	538	HIS	-	EXPRESSION TAG	UNP O33245
Z	539	HIS	-	EXPRESSION TAG	UNP O33245
Z	540	HIS	-	EXPRESSION TAG	UNP O33245
2	535	HIS	-	EXPRESSION TAG	UNP O33245
2	536	HIS	-	EXPRESSION TAG	UNP O33245
2	537	HIS	-	EXPRESSION TAG	UNP O33245
2	538	HIS	-	EXPRESSION TAG	UNP O33245
2	539	HIS	-	EXPRESSION TAG	UNP O33245
2	540	HIS	-	EXPRESSION TAG	UNP O33245

- Molecule 3 is N 2 -[(3R)-3-HYDROXYDODECANOYL]-L-ASPARAGINYL-N 1 -[(1S)-1-(HYDROXYMETHYL)-3-METHYLBUTYL]-L-GLUTAMAMIDE (three-letter code: FEB) (formula: C<sub>27</sub>H<sub>51</sub>N<sub>5</sub>O<sub>7</sub>).





Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	C	1	Total 32	C 20	N 5	O 7	0	0
3	E	1	Total 32	C 20	N 5	O 7	0	0
3	G	1	Total 32	C 20	N 5	O 7	0	0
3	H	1	Total 32	C 20	N 5	O 7	0	0
3	J	1	Total 32	C 20	N 5	O 7	0	0
3	L	1	Total 32	C 20	N 5	O 7	0	0
3	N	1	Total 32	C 20	N 5	O 7	0	0
3	P	1	Total 32	C 20	N 5	O 7	0	0
3	R	1	Total 32	C 20	N 5	O 7	0	0
3	T	1	Total 32	C 20	N 5	O 7	0	0
3	V	1	Total 32	C 20	N 5	O 7	0	0
3	X	1	Total 32	C 20	N 5	O 7	0	0
3	Z	1	Total 32	C 20	N 5	O 7	0	0
3	2	1	Total 32	C 20	N 5	O 7	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	32	Total O 32 32	0	0
4	B	42	Total O 42 42	0	0
4	C	131	Total O 131 131	0	0
4	D	25	Total O 25 25	0	0
4	E	130	Total O 130 130	0	0
4	F	41	Total O 41 41	0	0
4	G	113	Total O 113 113	0	0
4	H	126	Total O 126 126	0	0
4	I	38	Total O 38 38	0	0
4	J	122	Total O 122 122	0	0
4	K	33	Total O 33 33	0	0
4	L	132	Total O 132 132	0	0
4	M	42	Total O 42 42	0	0
4	N	121	Total O 121 121	0	0
4	O	39	Total O 39 39	0	0
4	P	111	Total O 111 111	0	0
4	Q	34	Total O 34 34	0	0
4	R	143	Total O 143 143	0	0
4	S	43	Total O 43 43	0	0
4	T	103	Total O 103 103	0	0
4	U	33	Total O 33 33	0	0

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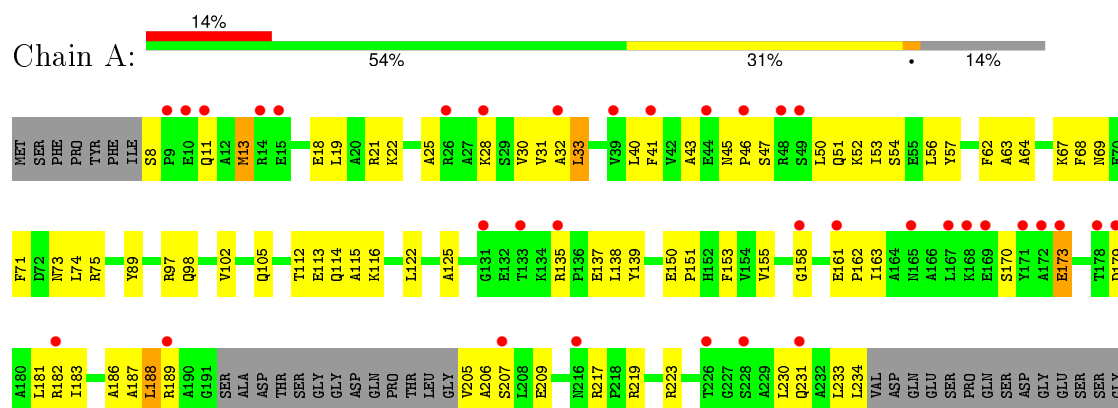
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	V	149	Total 149	O 149	0	0
4	W	26	Total 26	O 26	0	0
4	X	115	Total 115	O 115	0	0
4	Y	22	Total 22	O 22	0	0
4	Z	106	Total 106	O 106	0	0
4	1	55	Total 55	O 55	0	0
4	2	118	Total 118	O 118	0	0

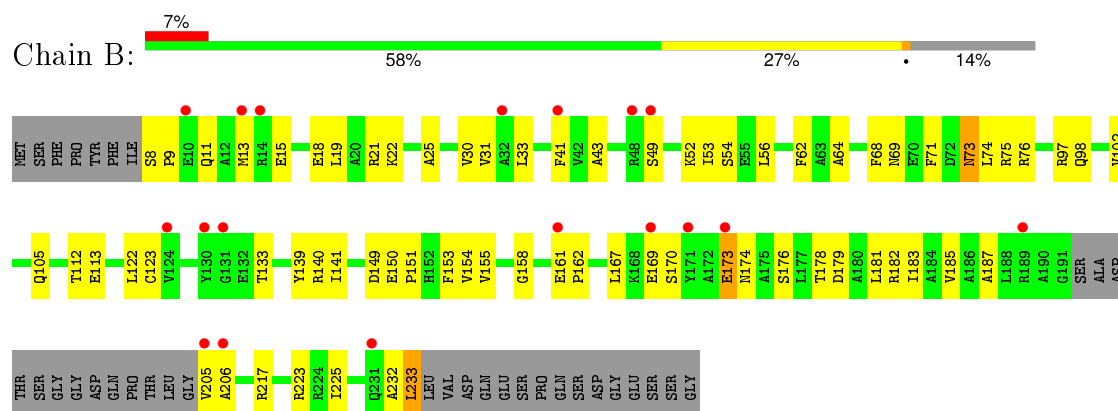
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

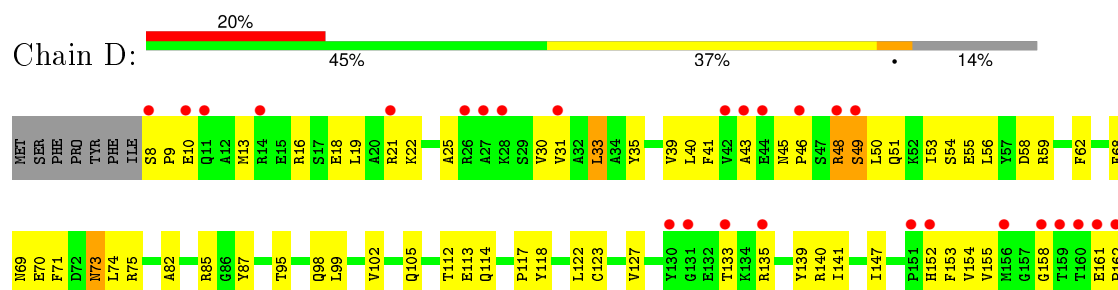
#### • Molecule 1: Proteasome subunit alpha

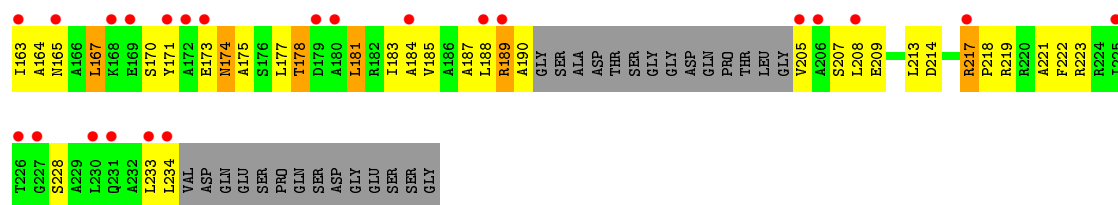


#### • Molecule 1: Proteasome subunit alpha

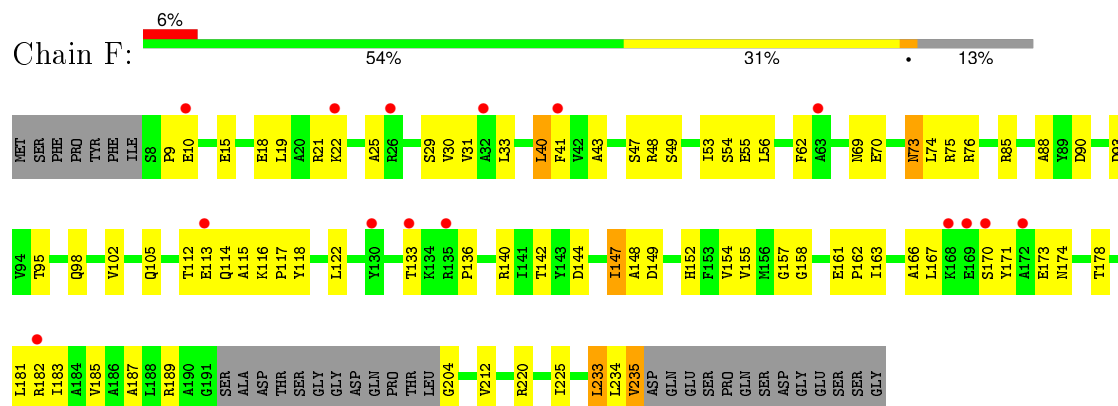


#### • Molecule 1: Proteasome subunit alpha

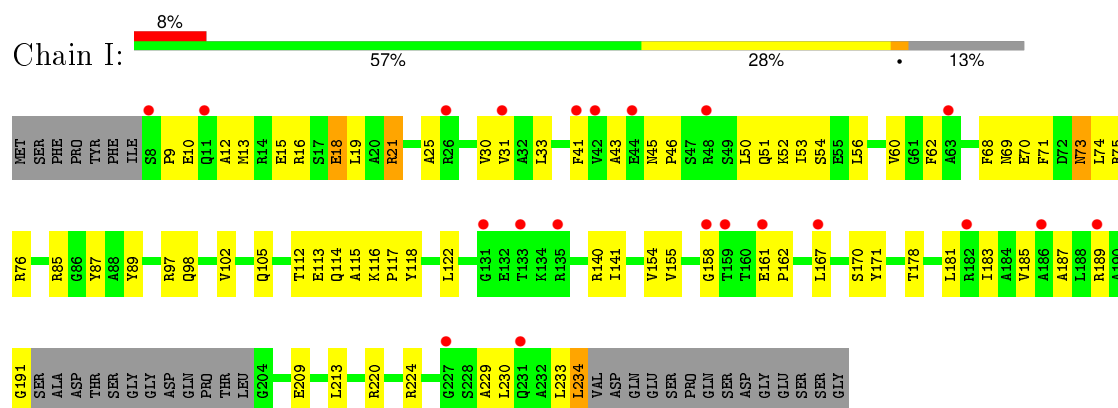




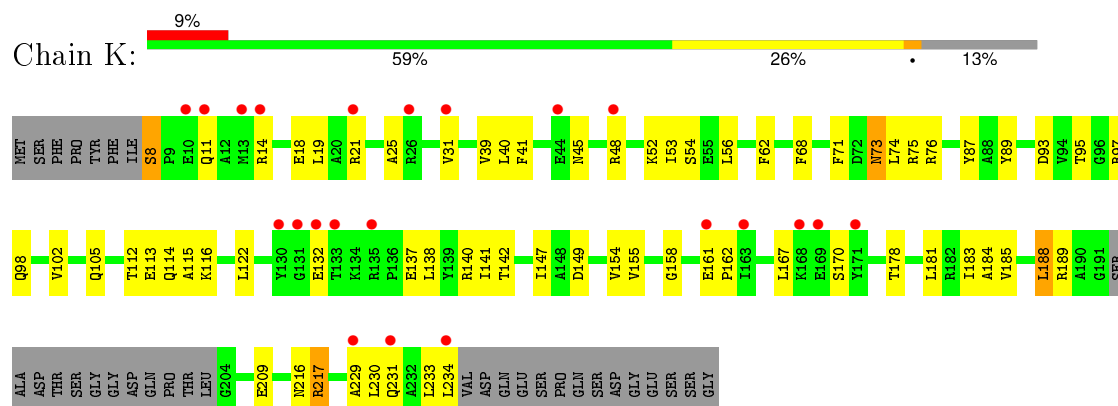
• Molecule 1: Proteasome subunit alpha



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• Molecule 1: Proteasome subunit alpha



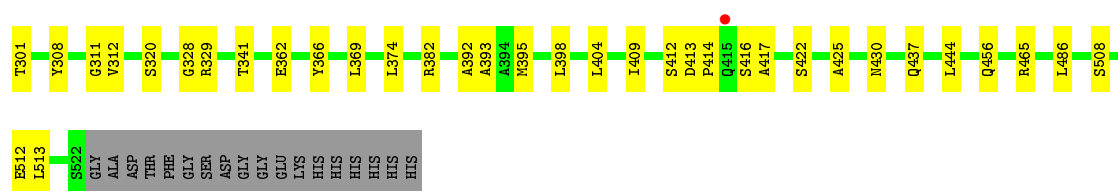
• Molecule 1: Proteasome subunit alpha



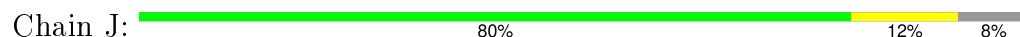




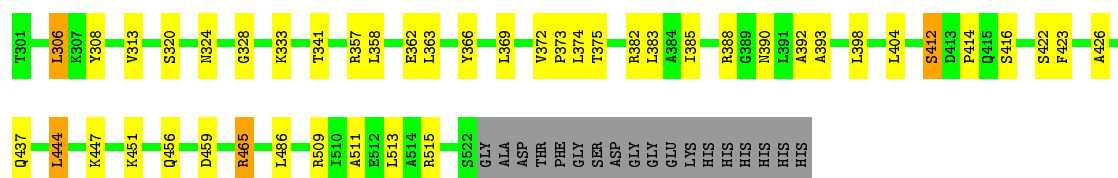




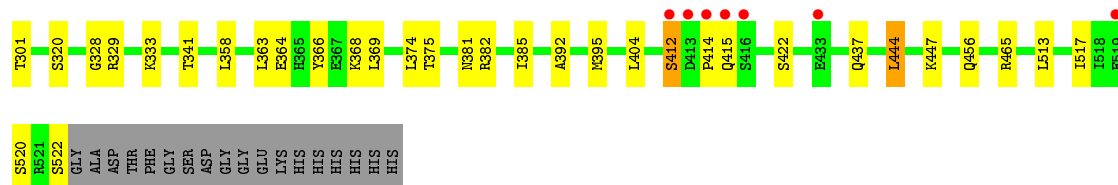
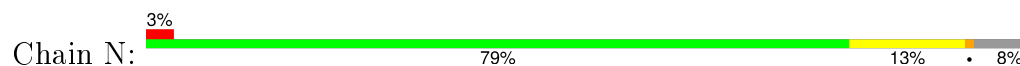
• Molecule 2: Proteasome subunit beta



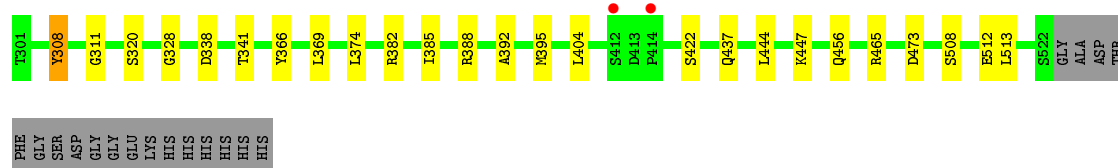
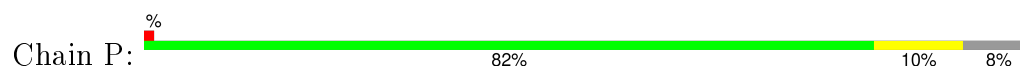
• Molecule 2: Proteasome subunit beta



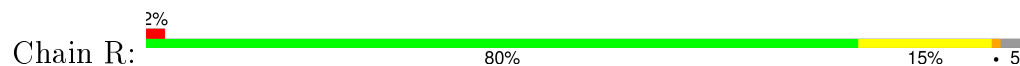
• Molecule 2: Proteasome subunit beta

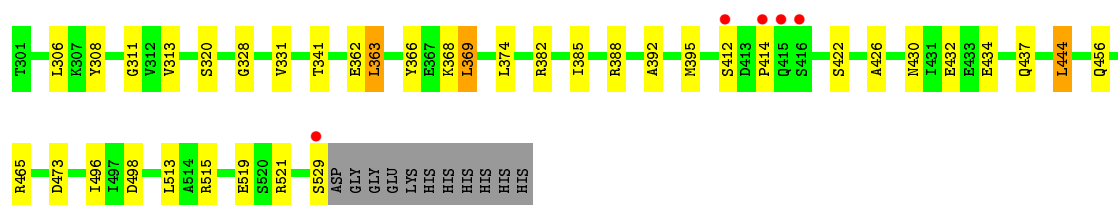


• Molecule 2: Proteasome subunit beta

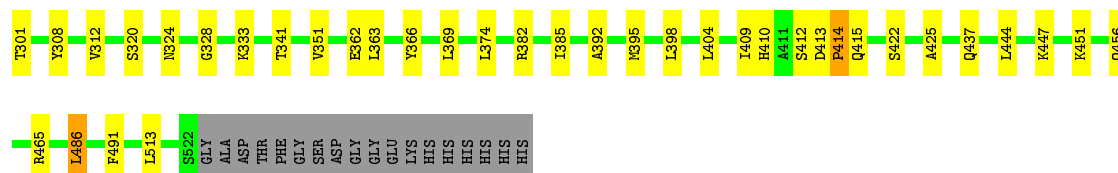


• Molecule 2: Proteasome subunit beta

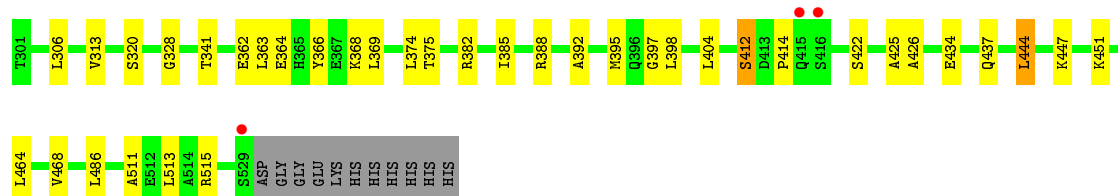
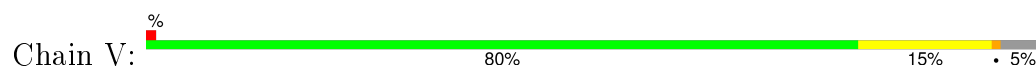




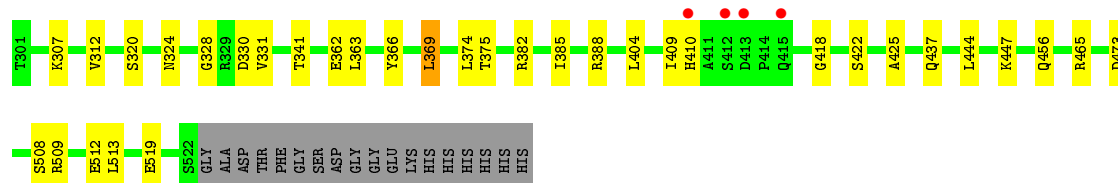
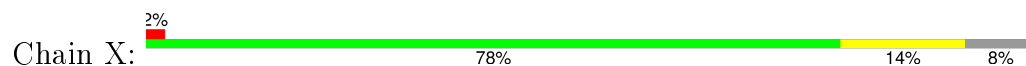
• Molecule 2: Proteasome subunit beta



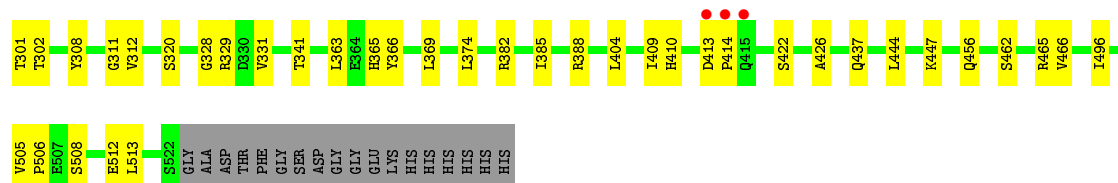
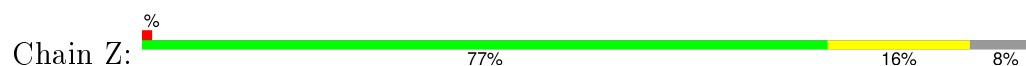
• Molecule 2: Proteasome subunit beta



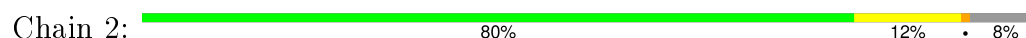
• Molecule 2: Proteasome subunit beta

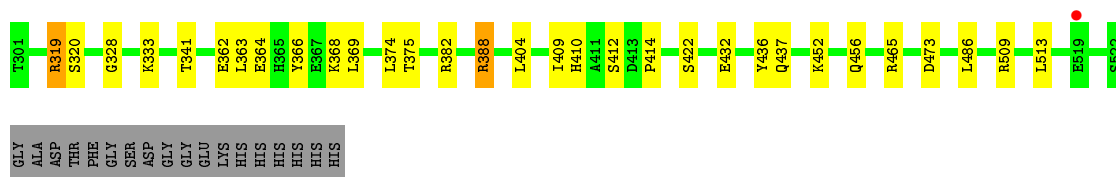


• Molecule 2: Proteasome subunit beta



• Molecule 2: Proteasome subunit beta





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	170.19Å 118.10Å 194.35Å 90.00° 112.62° 90.00°	Depositor
Resolution (Å)	25.00 – 2.50 25.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	96.5 (25.00-2.50) 96.6 (25.00-2.50)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	0.11	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.67 (at 2.50Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, $R_{free}$	0.208 , 0.229 0.207 , 0.226	Depositor DCC
$R_{free}$ test set	11782 reflections (4.99%)	DCC
Wilson B-factor (Å <sup>2</sup> )	30.7	Xtriage
Anisotropy	0.279	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 53.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	5 of 241958 reflections (0.002%)	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	48828	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.82% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: FEB

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	0.81	0/1679	0.76	0/2268
1	A	0.73	1/1675 (0.1%)	0.70	0/2263
1	B	0.62	0/1667	0.69	1/2252 (0.0%)
1	D	0.62	0/1671	0.79	1/2258 (0.0%)
1	F	0.70	0/1686	0.74	0/2278
1	I	0.67	0/1679	0.75	1/2268 (0.0%)
1	K	0.76	0/1679	0.77	0/2268
1	M	0.65	0/1675	0.71	0/2263
1	O	0.70	0/1675	0.76	0/2263
1	Q	0.69	0/1675	0.73	1/2263 (0.0%)
1	S	0.67	0/1682	0.73	2/2273 (0.1%)
1	U	0.66	0/1675	0.71	0/2263
1	W	0.56	0/1679	0.74	1/2268 (0.0%)
1	Y	0.73	0/1686	0.75	0/2278
2	2	0.77	0/1662	0.77	1/2254 (0.0%)
2	C	0.70	0/1662	0.78	2/2254 (0.1%)
2	E	0.76	0/1662	0.79	0/2254
2	G	0.70	0/1662	0.75	0/2254
2	H	0.73	0/1662	0.76	0/2254
2	J	0.75	0/1662	0.78	0/2254
2	L	0.74	1/1662 (0.1%)	0.77	1/2254 (0.0%)
2	N	0.66	0/1662	0.74	0/2254
2	P	0.76	1/1662 (0.1%)	0.76	2/2254 (0.1%)
2	R	0.82	0/1708	0.79	1/2316 (0.0%)
2	T	0.76	0/1662	0.82	0/2254
2	V	0.82	0/1708	0.75	0/2316
2	X	0.70	0/1662	0.78	1/2254 (0.0%)
2	Z	0.63	0/1662	0.76	1/2254 (0.0%)
All	All	0.71	3/46843 (0.0%)	0.75	16/63406 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	308	TYR	CD1-CE1	-5.57	1.30	1.39
2	P	308	TYR	CD1-CE1	-5.11	1.31	1.39
1	A	57	TYR	CD1-CE1	-5.10	1.31	1.39

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S	183	ILE	CB-CA-C	-5.96	99.67	111.60
1	Q	183	ILE	CB-CA-C	-5.70	100.20	111.60
2	C	413	ASP	C-N-CD	-5.67	108.12	120.60
2	Z	388	ARG	NE-CZ-NH2	-5.42	117.59	120.30
2	2	388	ARG	NE-CZ-NH2	-5.37	117.61	120.30

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	1	1654	0	1651	93	0
1	A	1650	0	1648	74	0
1	B	1642	0	1637	64	0
1	D	1646	0	1645	144	0
1	F	1661	0	1660	68	0
1	I	1654	0	1651	62	0
1	K	1654	0	1651	82	0
1	M	1650	0	1648	69	0
1	O	1650	0	1648	96	0
1	Q	1650	0	1648	89	0
1	S	1657	0	1657	98	0
1	U	1650	0	1648	64	0
1	W	1654	0	1651	90	0
1	Y	1661	0	1660	120	0
2	2	1638	0	1629	26	0
2	C	1638	0	1629	36	0
2	E	1638	0	1629	30	0
2	G	1638	0	1629	34	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	H	1638	0	1629	22	0
2	J	1638	0	1629	30	0
2	L	1638	0	1629	49	0
2	N	1638	0	1629	24	0
2	P	1638	0	1629	18	0
2	R	1683	0	1665	37	0
2	T	1638	0	1629	37	0
2	V	1683	0	1665	31	0
2	X	1638	0	1629	27	0
2	Z	1638	0	1629	24	0
3	2	32	0	33	2	0
3	C	32	0	33	3	0
3	E	32	0	33	2	0
3	G	32	0	33	3	0
3	H	32	0	33	1	0
3	J	32	0	33	1	0
3	L	32	0	33	1	0
3	N	32	0	33	3	0
3	P	32	0	33	2	0
3	R	32	0	33	3	0
3	T	32	0	33	3	0
3	V	32	0	33	0	0
3	X	32	0	33	2	0
3	Z	32	0	33	2	0
4	1	55	0	0	2	0
4	2	118	0	0	6	0
4	A	32	0	0	3	0
4	B	42	0	0	3	0
4	C	131	0	0	11	0
4	D	25	0	0	3	0
4	E	130	0	0	7	0
4	F	41	0	0	6	0
4	G	113	0	0	8	0
4	H	126	0	0	6	0
4	I	38	0	0	6	0
4	J	122	0	0	3	0
4	K	33	0	0	6	0
4	L	132	0	0	9	0
4	M	42	0	0	0	0
4	N	121	0	0	3	0
4	O	39	0	0	6	0
4	P	111	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	Q	34	0	0	0	0
4	R	143	0	0	9	0
4	S	43	0	0	19	0
4	T	103	0	0	3	0
4	U	33	0	0	2	0
4	V	149	0	0	5	0
4	W	26	0	0	3	0
4	X	115	0	0	4	0
4	Y	22	0	0	3	0
4	Z	106	0	0	1	0
All	All	48828	0	46443	1514	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 16.

The worst 5 of 1514 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)
1:D:217:ARG:NH1	1:D:217:ARG:HB2	1.41	1.30
1:A:13:MET:CE	1:O:116:LYS:HD3	1.62	1.27
1:M:217:ARG:HD3	1:M:223:ARG:NH2	1.53	1.24
1:B:170:SER:OG	1:B:183:ILE:HG23	1.39	1.23
1:Y:229:ALA:O	1:Y:233:LEU:HD13	1.41	1.20

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	1	211/248 (85%)	199 (94%)	11 (5%)	1 (0%)	34 55
1	A	210/248 (85%)	203 (97%)	7 (3%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	209/248 (84%)	203 (97%)	6 (3%)	0	100	100
1	D	209/248 (84%)	203 (97%)	6 (3%)	0	100	100
1	F	212/248 (86%)	208 (98%)	4 (2%)	0	100	100
1	I	211/248 (85%)	208 (99%)	3 (1%)	0	100	100
1	K	211/248 (85%)	204 (97%)	7 (3%)	0	100	100
1	M	210/248 (85%)	204 (97%)	6 (3%)	0	100	100
1	O	210/248 (85%)	203 (97%)	7 (3%)	0	100	100
1	Q	210/248 (85%)	202 (96%)	8 (4%)	0	100	100
1	S	211/248 (85%)	204 (97%)	7 (3%)	0	100	100
1	U	210/248 (85%)	206 (98%)	4 (2%)	0	100	100
1	W	211/248 (85%)	205 (97%)	6 (3%)	0	100	100
1	Y	212/248 (86%)	206 (97%)	6 (3%)	0	100	100
2	2	220/240 (92%)	220 (100%)	0	0	100	100
2	C	220/240 (92%)	220 (100%)	0	0	100	100
2	E	220/240 (92%)	218 (99%)	2 (1%)	0	100	100
2	G	220/240 (92%)	218 (99%)	2 (1%)	0	100	100
2	H	220/240 (92%)	217 (99%)	3 (1%)	0	100	100
2	J	220/240 (92%)	218 (99%)	2 (1%)	0	100	100
2	L	220/240 (92%)	218 (99%)	2 (1%)	0	100	100
2	N	220/240 (92%)	218 (99%)	2 (1%)	0	100	100
2	P	220/240 (92%)	218 (99%)	2 (1%)	0	100	100
2	R	227/240 (95%)	224 (99%)	3 (1%)	0	100	100
2	T	220/240 (92%)	219 (100%)	1 (0%)	0	100	100
2	V	227/240 (95%)	226 (100%)	1 (0%)	0	100	100
2	X	220/240 (92%)	219 (100%)	1 (0%)	0	100	100
2	Z	220/240 (92%)	217 (99%)	3 (1%)	0	100	100
All	All	6041/6832 (88%)	5928 (98%)	112 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1	131	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	1	164/192 (85%)	151 (92%)	13 (8%)	15	28
1	A	164/192 (85%)	160 (98%)	4 (2%)	57	82
1	B	163/192 (85%)	158 (97%)	5 (3%)	47	75
1	D	164/192 (85%)	152 (93%)	12 (7%)	17	32
1	F	165/192 (86%)	153 (93%)	12 (7%)	17	32
1	I	164/192 (85%)	157 (96%)	7 (4%)	35	61
1	K	164/192 (85%)	156 (95%)	8 (5%)	31	55
1	M	164/192 (85%)	154 (94%)	10 (6%)	23	42
1	O	164/192 (85%)	151 (92%)	13 (8%)	15	28
1	Q	164/192 (85%)	154 (94%)	10 (6%)	23	42
1	S	165/192 (86%)	158 (96%)	7 (4%)	36	62
1	U	164/192 (85%)	159 (97%)	5 (3%)	48	76
1	W	164/192 (85%)	159 (97%)	5 (3%)	48	76
1	Y	165/192 (86%)	156 (94%)	9 (6%)	27	48
2	2	165/178 (93%)	160 (97%)	5 (3%)	48	76
2	C	165/178 (93%)	161 (98%)	4 (2%)	57	82
2	E	165/178 (93%)	161 (98%)	4 (2%)	57	82
2	G	165/178 (93%)	160 (97%)	5 (3%)	48	76
2	H	165/178 (93%)	158 (96%)	7 (4%)	36	62
2	J	165/178 (93%)	160 (97%)	5 (3%)	48	76
2	L	165/178 (93%)	155 (94%)	10 (6%)	23	42
2	N	165/178 (93%)	159 (96%)	6 (4%)	42	69
2	P	165/178 (93%)	163 (99%)	2 (1%)	78	93
2	R	169/178 (95%)	163 (96%)	6 (4%)	42	69
2	T	165/178 (93%)	157 (95%)	8 (5%)	31	55
2	V	169/178 (95%)	163 (96%)	6 (4%)	42	69

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	X	165/178 (93%)	159 (96%)	6 (4%)	42	69
2	Z	165/178 (93%)	159 (96%)	6 (4%)	42	69
All	All	4616/5180 (89%)	4416 (96%)	200 (4%)	35	61

5 of 200 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	M	223	ARG
1	O	223	ARG
1	1	97	ARG
2	N	363	LEU
1	O	48	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 114 such sidechains are listed below:

Mol	Chain	Res	Type
1	O	69	ASN
1	Q	174	ASN
1	1	69	ASN
1	O	105	GLN
2	P	324	ASN

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

14 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	FEB	2	300	2	31,31,38	1.18	3 (9%)	39,40,47	1.27	4 (10%)
3	FEB	C	300	2	31,31,38	1.11	3 (9%)	39,40,47	1.25	5 (12%)
3	FEB	E	300	2	31,31,38	1.14	2 (6%)	39,40,47	1.15	2 (5%)
3	FEB	G	300	2	31,31,38	1.27	5 (16%)	39,40,47	1.30	5 (12%)
3	FEB	H	300	2	31,31,38	1.37	7 (22%)	39,40,47	1.21	5 (12%)
3	FEB	J	300	2	31,31,38	1.31	3 (9%)	39,40,47	1.28	5 (12%)
3	FEB	L	300	2	31,31,38	1.27	5 (16%)	39,40,47	1.22	4 (10%)
3	FEB	N	300	2	31,31,38	1.32	4 (12%)	39,40,47	1.25	5 (12%)
3	FEB	P	300	2	31,31,38	1.34	5 (16%)	39,40,47	1.32	4 (10%)
3	FEB	R	300	2	31,31,38	1.22	3 (9%)	39,40,47	1.25	4 (10%)
3	FEB	T	300	2	31,31,38	1.29	4 (12%)	39,40,47	1.34	5 (12%)
3	FEB	V	300	2	31,31,38	1.33	4 (12%)	39,40,47	1.20	5 (12%)
3	FEB	X	300	2	31,31,38	1.21	4 (12%)	39,40,47	1.26	6 (15%)
3	FEB	Z	300	2	31,31,38	1.15	3 (9%)	39,40,47	1.29	7 (17%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	FEB	2	300	2	-	0/41/41/48	0/0/0/0
3	FEB	C	300	2	-	0/41/41/48	0/0/0/0
3	FEB	E	300	2	-	0/41/41/48	0/0/0/0
3	FEB	G	300	2	-	0/41/41/48	0/0/0/0
3	FEB	H	300	2	-	0/41/41/48	0/0/0/0
3	FEB	J	300	2	-	0/41/41/48	0/0/0/0
3	FEB	L	300	2	-	0/41/41/48	0/0/0/0
3	FEB	N	300	2	-	0/41/41/48	0/0/0/0
3	FEB	P	300	2	-	0/41/41/48	0/0/0/0
3	FEB	R	300	2	-	0/41/41/48	0/0/0/0
3	FEB	T	300	2	-	0/41/41/48	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	FEB	V	300	2	-	0/41/41/48	0/0/0/0
3	FEB	X	300	2	-	0/41/41/48	0/0/0/0
3	FEB	Z	300	2	-	0/41/41/48	0/0/0/0

The worst 5 of 55 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	T	300	FEB	C36-C38	2.01	1.55	1.51
3	H	300	FEB	O21-C20	2.02	1.27	1.23
3	C	300	FEB	O49-C38	2.02	1.27	1.23
3	E	300	FEB	O49-C38	2.02	1.27	1.23
3	H	300	FEB	C19-C20	2.06	1.58	1.52

The worst 5 of 66 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	2	300	FEB	C19-C20-N9	-3.04	109.77	116.78
3	X	300	FEB	C19-C20-N9	-3.03	109.79	116.78
3	T	300	FEB	C19-C20-N9	-3.03	109.79	116.78
3	J	300	FEB	C19-C20-N9	-3.00	109.87	116.78
3	P	300	FEB	C19-C20-N9	-2.96	109.95	116.78

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

13 monomers are involved in 28 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	2	300	FEB	2	0
3	C	300	FEB	3	0
3	E	300	FEB	2	0
3	G	300	FEB	3	0
3	H	300	FEB	1	0
3	J	300	FEB	1	0
3	L	300	FEB	1	0
3	N	300	FEB	3	0
3	P	300	FEB	2	0
3	R	300	FEB	3	0
3	T	300	FEB	3	0
3	X	300	FEB	2	0
3	Z	300	FEB	2	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	1	215/248 (86%)	0.53	24 (11%) 7 7	23, 51, 86, 94	0
1	A	214/248 (86%)	0.69	35 (16%) 2 2	24, 53, 88, 100	0
1	B	213/248 (85%)	0.61	18 (8%) 13 14	24, 52, 87, 94	0
1	D	213/248 (85%)	1.06	50 (23%) 1 1	25, 55, 93, 112	0
1	F	216/248 (87%)	0.53	15 (6%) 20 22	23, 53, 87, 93	0
1	I	215/248 (86%)	0.60	21 (9%) 10 10	24, 52, 87, 95	0
1	K	215/248 (86%)	0.49	22 (10%) 9 9	24, 53, 87, 95	0
1	M	214/248 (86%)	0.64	24 (11%) 7 7	23, 54, 88, 96	0
1	O	214/248 (86%)	0.63	24 (11%) 7 7	22, 53, 88, 95	0
1	Q	214/248 (86%)	0.71	25 (11%) 6 6	26, 52, 87, 95	0
1	S	215/248 (86%)	0.77	37 (17%) 2 2	24, 53, 89, 99	0
1	U	214/248 (86%)	0.67	29 (13%) 4 4	23, 53, 87, 95	0
1	W	215/248 (86%)	0.75	32 (14%) 3 3	24, 54, 93, 98	0
1	Y	216/248 (87%)	0.83	40 (18%) 2 2	26, 55, 90, 98	0
2	2	222/240 (92%)	-0.31	1 (0%) 91 92	12, 23, 41, 66	0
2	C	222/240 (92%)	-0.31	4 (1%) 71 75	13, 24, 41, 68	0
2	E	222/240 (92%)	-0.34	1 (0%) 91 92	13, 24, 41, 65	0
2	G	222/240 (92%)	-0.29	5 (2%) 64 67	14, 24, 43, 68	0
2	H	222/240 (92%)	-0.33	1 (0%) 91 92	11, 24, 42, 66	0
2	J	222/240 (92%)	-0.30	0 100 100	12, 24, 43, 65	0
2	L	222/240 (92%)	-0.34	0 100 100	13, 24, 42, 65	0
2	N	222/240 (92%)	-0.24	7 (3%) 51 56	13, 24, 43, 67	0
2	P	222/240 (92%)	-0.33	2 (0%) 85 88	14, 24, 42, 67	0
2	R	229/240 (95%)	-0.34	5 (2%) 65 69	13, 24, 46, 67	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
2	T	222/240 (92%)	-0.31	0 100 100	15, 25, 43, 67	0
2	V	229/240 (95%)	-0.34	3 (1%) 79 82	12, 23, 44, 67	0
2	X	222/240 (92%)	-0.34	4 (1%) 71 75	13, 25, 43, 67	0
2	Z	222/240 (92%)	-0.28	3 (1%) 78 80	13, 25, 43, 67	0
All	All	6125/6832 (89%)	0.17	432 (7%) 19 21	11, 35, 84, 112	0

The worst 5 of 432 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	233	LEU	7.3
1	B	205	VAL	6.7
1	Y	12	ALA	6.7
1	Y	10	GLU	6.6
1	S	235	VAL	5.3

## 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 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
3	FEB	Z	300	32/39	0.93	0.15	2.36	23,29,36,37	0
3	FEB	X	300	32/39	0.92	0.15	1.83	21,26,30,33	0
3	FEB	T	300	32/39	0.94	0.13	1.29	18,27,36,37	0
3	FEB	L	300	32/39	0.95	0.14	1.20	18,24,34,37	0
3	FEB	R	300	32/39	0.94	0.15	1.19	21,25,37,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	FEB	E	300	32/39	0.93	0.14	1.15	10,21,35,37	0
3	FEB	P	300	32/39	0.95	0.13	1.03	20,26,35,37	0
3	FEB	C	300	32/39	0.95	0.14	1.00	19,25,32,35	0
3	FEB	J	300	32/39	0.94	0.12	0.99	12,23,36,38	0
3	FEB	H	300	32/39	0.94	0.14	0.97	17,25,34,38	0
3	FEB	G	300	32/39	0.95	0.14	0.69	17,25,32,34	0
3	FEB	N	300	32/39	0.94	0.13	0.68	15,25,33,36	0
3	FEB	2	300	32/39	0.93	0.14	0.61	16,27,34,34	0
3	FEB	V	300	32/39	0.95	0.12	0.24	17,27,36,37	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.