



wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 18, 2026 – 02:58 PM UTC

PDB ID : 3MFE / pdb_00003mfe
Title : Crystal Structure of Mycobacterium Tuberculosis Proteasome open-gate mutant with H0 movement
Authors : Li, D.; Li, H.
Deposited on : 2010-04-02
Resolution : 2.60 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
Mogul : 2022.3.0, CSD as543be (2022)
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

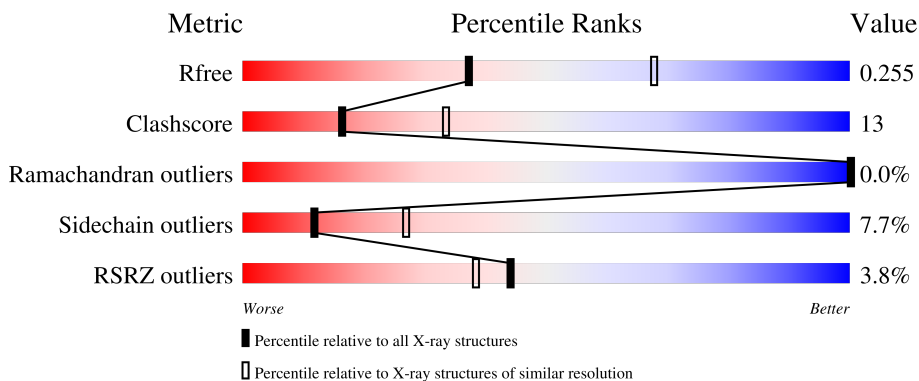
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION



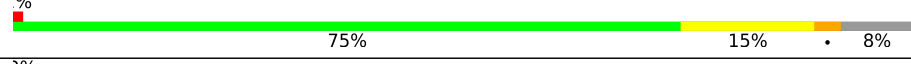
The reported resolution of this entry is 2.60 Å.

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.



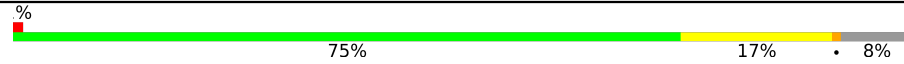

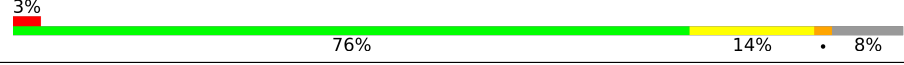



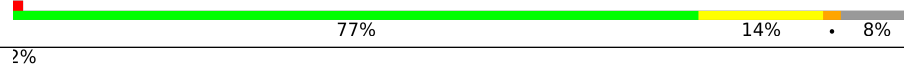

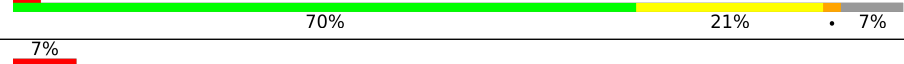


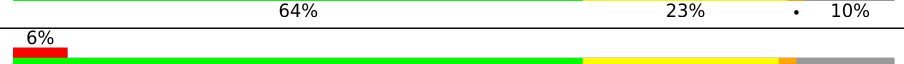

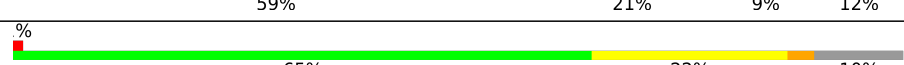

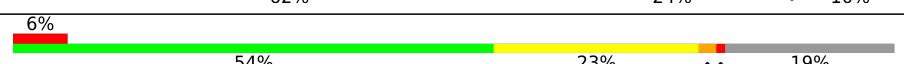
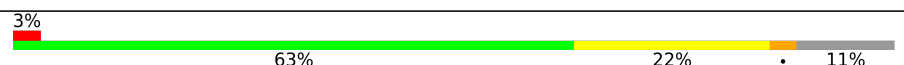
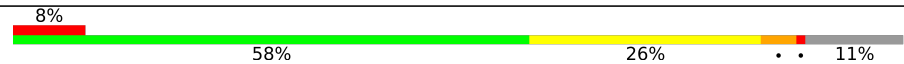
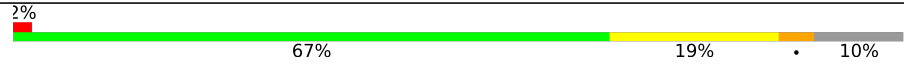



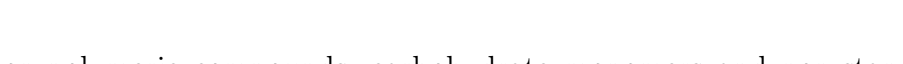
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	2	240	 79% 12% • 8%
1	C	240	 73% 17% • 8%
1	E	240	 75% 15% • 8%
1	H	240	 77% 12% • 8%
1	J	240	 78% 12% • 8%

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Mol	Chain	Length	Quality of chain
1	L	240	
1	N	240	
1	P	240	
1	R	240	
1	T	240	
1	X	240	
1	Z	240	
2	G	240	
2	V	240	
3	I	240	
3	A	240	
3	B	240	
3	D	240	
3	F	240	
3	I	240	
3	K	240	
3	M	240	
3	O	240	
3	Q	240	
3	S	240	
3	U	240	
3	W	240	
3	Y	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
1	OZT	2	301	-	-	X	-
1	OZT	C	301	-	-	X	-
1	OZT	E	301	-	-	X	-
1	OZT	H	301	-	-	X	-
1	OZT	J	301	-	-	X	-
1	OZT	L	301	-	-	X	-
1	OZT	P	301	-	-	X	-
1	OZT	R	301	-	-	X	-
1	OZT	T	301	-	-	X	-
1	OZT	X	301	-	-	X	-
1	OZT	Z	301	-	-	X	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 46890 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 beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	H	222	Total 1640	C 1028	N 282	O 325	S 5	0	0	0
1	C	222	Total 1640	C 1028	N 282	O 325	S 5	0	0	0
1	E	222	Total 1640	C 1028	N 282	O 325	S 5	0	0	0
1	J	222	Total 1640	C 1028	N 282	O 325	S 5	0	0	0
1	L	222	Total 1640	C 1028	N 282	O 325	S 5	0	0	0
1	N	222	Total 1640	C 1028	N 282	O 325	S 5	0	0	0
1	P	222	Total 1640	C 1028	N 282	O 325	S 5	0	0	0
1	R	222	Total 1640	C 1028	N 282	O 325	S 5	0	0	0
1	T	222	Total 1640	C 1028	N 282	O 325	S 5	0	0	0
1	X	222	Total 1640	C 1028	N 282	O 325	S 5	0	0	0
1	Z	222	Total 1640	C 1028	N 282	O 325	S 5	0	0	0
1	2	222	Total 1640	C 1028	N 282	O 325	S 5	0	0	0

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	301	OZT	-	amidation	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

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Chain	Residue	Modelled	Actual	Comment	Reference
H	539	HIS	-	expression tag	UNP O33245
H	540	HIS	-	expression tag	UNP O33245
C	301	OZT	-	amidation	UNP O33245
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	301	OZT	-	amidation	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
J	301	OZT	-	amidation	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	301	OZT	-	amidation	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	301	OZT	-	amidation	UNP O33245
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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	301	OZT	-	amidation	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

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Chain	Residue	Modelled	Actual	Comment	Reference
P	539	HIS	-	expression tag	UNP O33245
P	540	HIS	-	expression tag	UNP O33245
R	301	OZT	-	amidation	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
T	301	OZT	-	amidation	UNP O33245
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
X	301	OZT	-	amidation	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	301	OZT	-	amidation	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	301	OZT	-	amidation	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 2 is a protein called Proteasome subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	G	222	1638	1027	282	324	5	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	V	224	1647	1032	284	326	5	0	0	0

There are 12 discrepancies between the modelled and reference sequences:

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
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

- Molecule 3 is a protein called Proteasome subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	D	213	1643	1028	301	311	3	0	0	0
3	A	214	1651	1033	302	312	4	0	0	0
3	B	216	1662	1040	304	314	4	0	0	0
3	F	212	1634	1023	300	308	3	0	0	0
3	I	217	1670	1046	305	315	4	0	0	0
3	K	216	1662	1041	304	314	3	0	0	0
3	M	194	1489	935	268	284	2	0	0	0
3	O	214	1650	1033	302	312	3	0	0	0
3	Q	213	1643	1028	301	311	3	0	0	0
3	S	215	1658	1038	303	313	4	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	U	212	Total	C	N	O	S	0	0	0
			1637	1025	300	309	3			
3	W	209	Total	C	N	O	S	0	0	0
			1612	1010	296	304	2			
3	Y	213	Total	C	N	O	S	0	0	0
			1643	1028	301	311	3			
3	1	213	Total	C	N	O	S	0	0	0
			1643	1028	301	311	3			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	9	MET	-	initiating methionine	UNP O33244
A	9	MET	-	initiating methionine	UNP O33244
B	9	MET	-	initiating methionine	UNP O33244
F	9	MET	-	initiating methionine	UNP O33244
I	9	MET	-	initiating methionine	UNP O33244
K	9	MET	-	initiating methionine	UNP O33244
M	9	MET	-	initiating methionine	UNP O33244
O	9	MET	-	initiating methionine	UNP O33244
Q	9	MET	-	initiating methionine	UNP O33244
S	9	MET	-	initiating methionine	UNP O33244
U	9	MET	-	initiating methionine	UNP O33244
W	9	MET	-	initiating methionine	UNP O33244
Y	9	MET	-	initiating methionine	UNP O33244
1	9	MET	-	initiating methionine	UNP O33244

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	H	42	Total	O	0	0
			42	42		
4	C	33	Total	O	0	0
			33	33		
4	E	38	Total	O	0	0
			38	38		
4	G	41	Total	O	0	0
			41	41		
4	J	33	Total	O	0	0
			33	33		
4	L	43	Total	O	0	0
			43	43		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	N	74	Total O 74 74	0	0
4	P	68	Total O 68 68	0	0
4	R	41	Total O 41 41	0	0
4	T	34	Total O 34 34	0	0
4	V	70	Total O 70 70	0	0
4	X	51	Total O 51 51	0	0
4	Z	35	Total O 35 35	0	0
4	2	45	Total O 45 45	0	0
4	D	18	Total O 18 18	0	0
4	A	36	Total O 36 36	0	0
4	B	46	Total O 46 46	0	0
4	F	33	Total O 33 33	0	0
4	I	39	Total O 39 39	0	0
4	K	30	Total O 30 30	0	0
4	M	19	Total O 19 19	0	0
4	O	33	Total O 33 33	0	0
4	Q	13	Total O 13 13	0	0
4	S	19	Total O 19 19	0	0
4	U	31	Total O 31 31	0	0
4	W	18	Total O 18 18	0	0
4	Y	23	Total O 23 23	0	0

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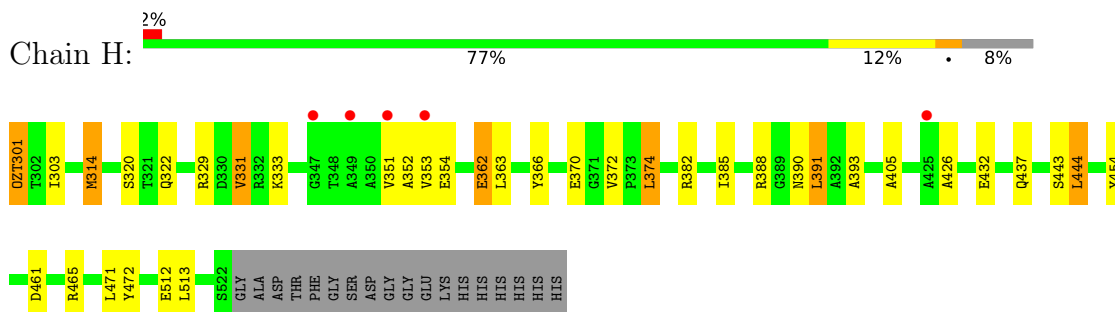
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	1	22	Total	O	0	0
			22	22		

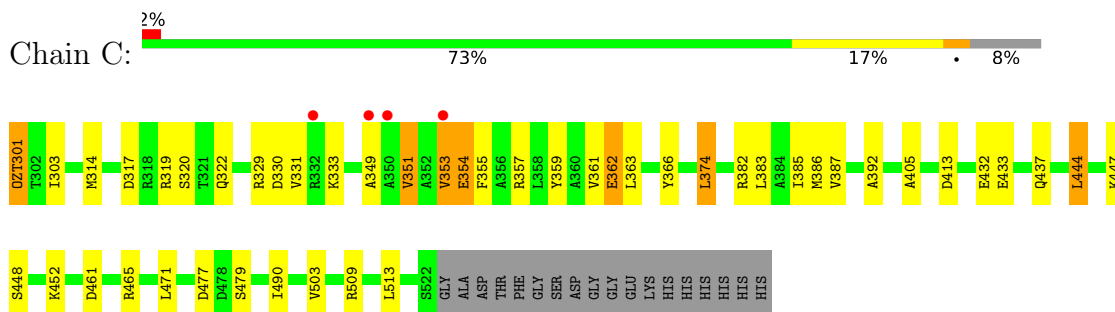
3 Residue-property plots [i](#)

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.

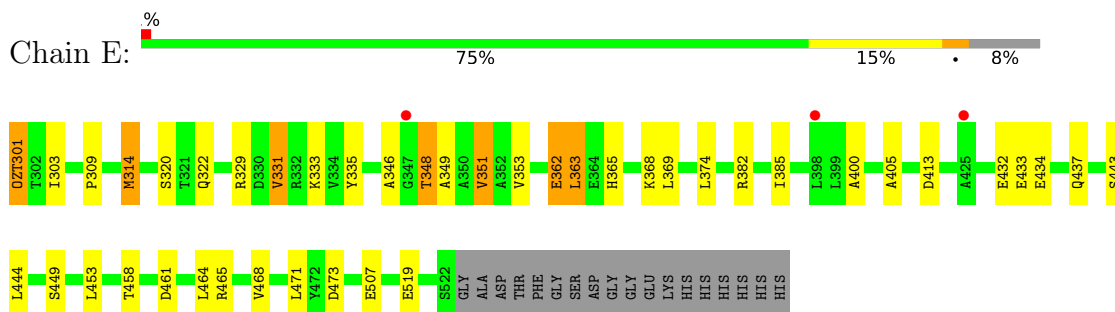
- Molecule 1: Proteasome subunit beta



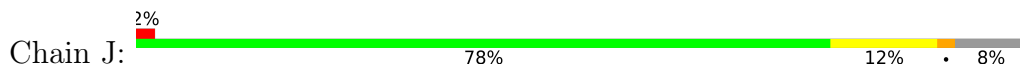
- Molecule 1: Proteasome subunit beta

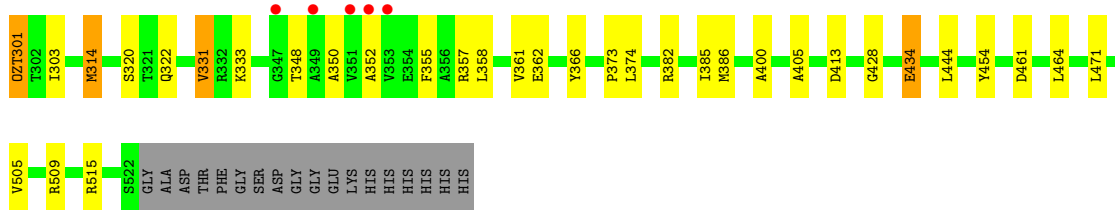


- Molecule 1: Proteasome subunit beta

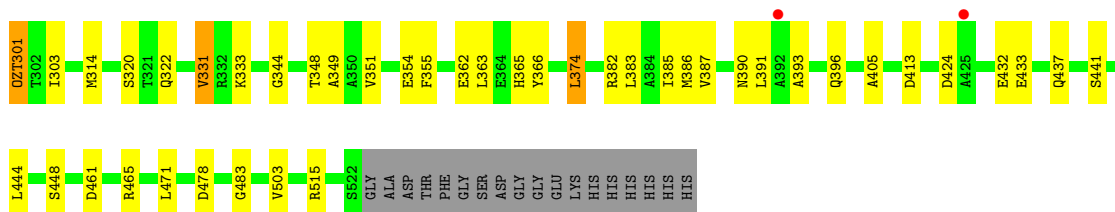
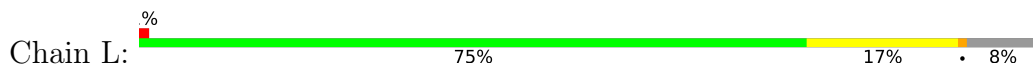


- Molecule 1: Proteasome subunit beta

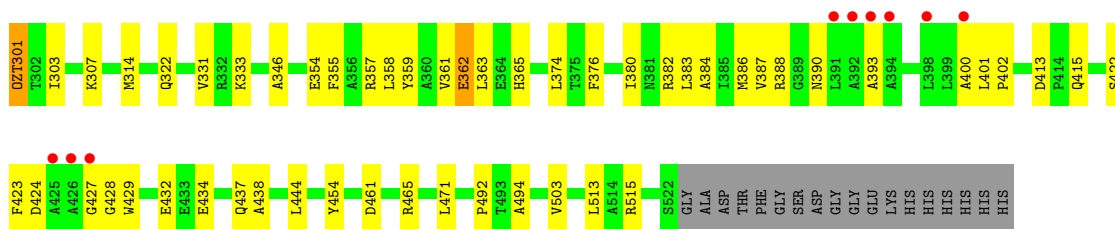




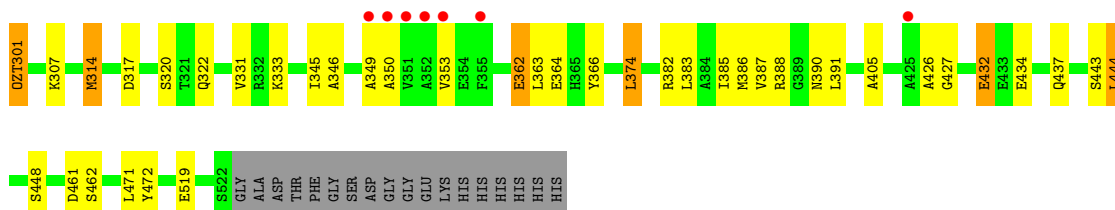
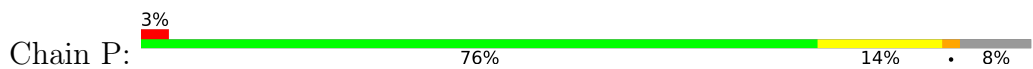
• Molecule 1: Proteasome subunit beta



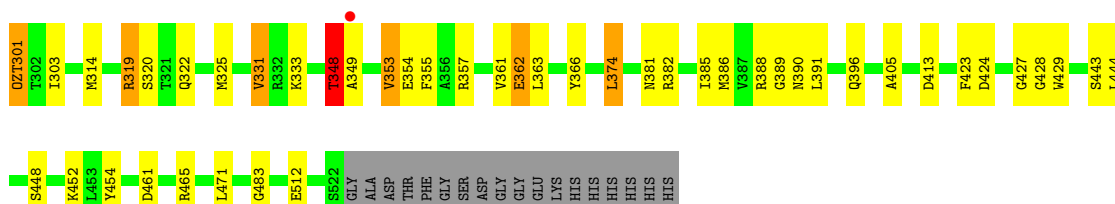
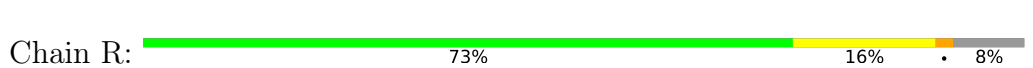
• Molecule 1: Proteasome subunit beta

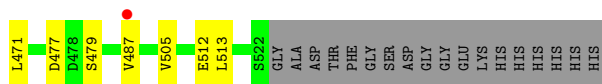


• Molecule 1: Proteasome subunit beta

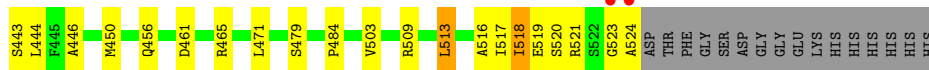


• Molecule 1: Proteasome subunit beta

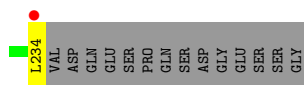




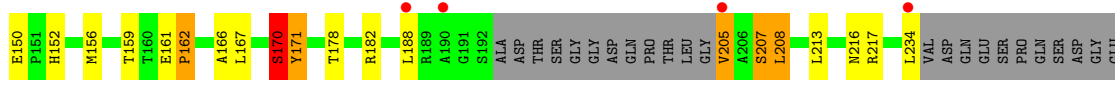
• Molecule 2: Proteasome subunit beta



• Molecule 3: Proteasome subunit alpha

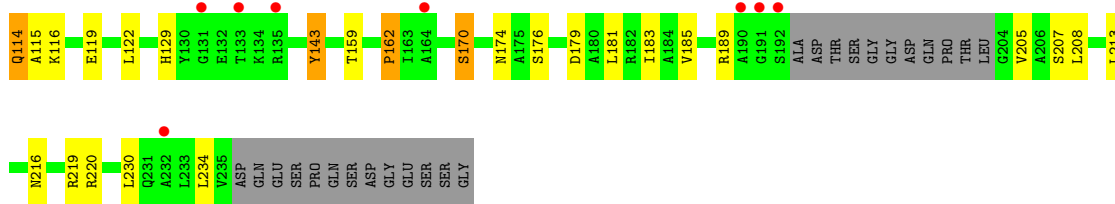


• Molecule 3: Proteasome subunit alpha

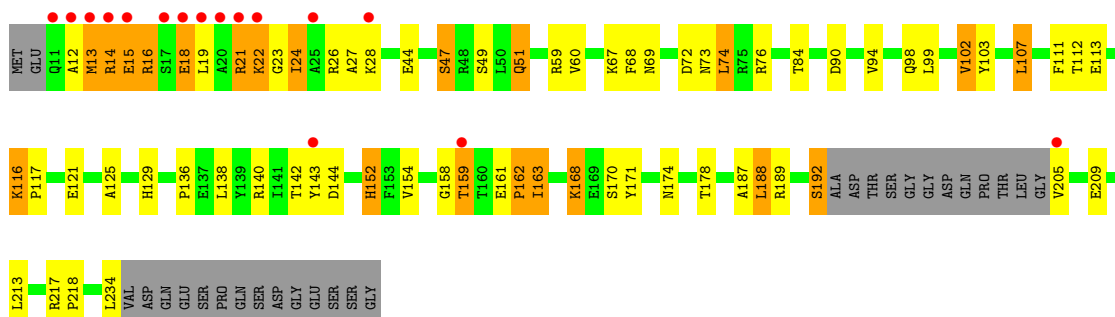


• Molecule 3: Proteasome subunit alpha

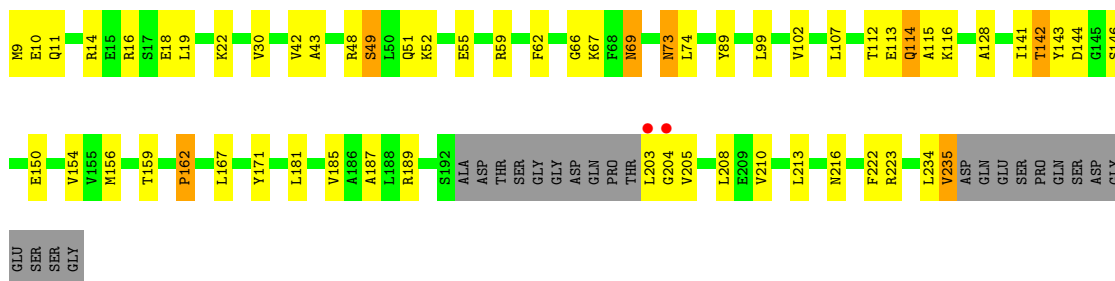




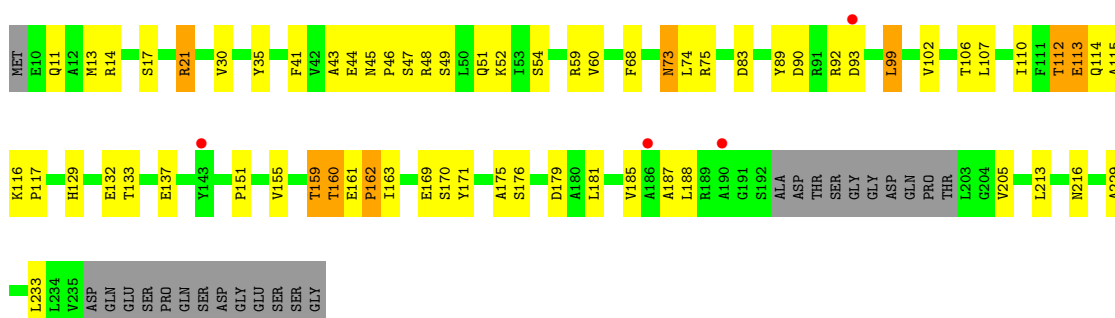
• Molecule 3: Proteasome subunit alpha



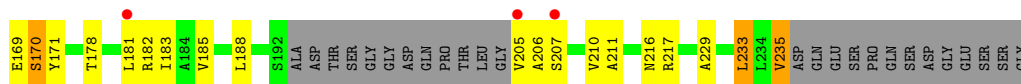
• Molecule 3: Proteasome subunit alpha



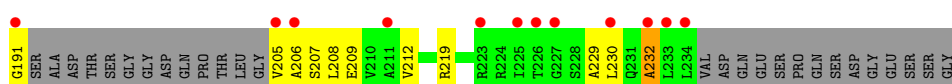
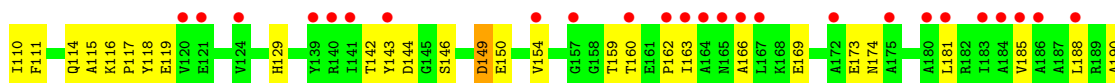
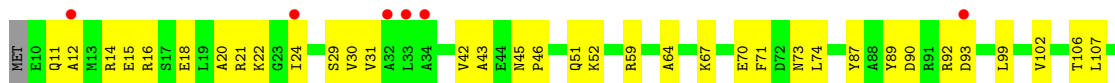
• Molecule 3: Proteasome subunit alpha



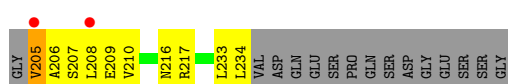
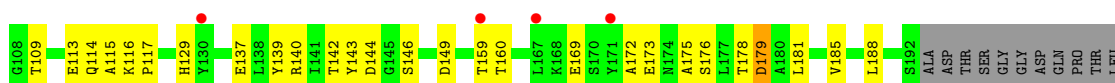
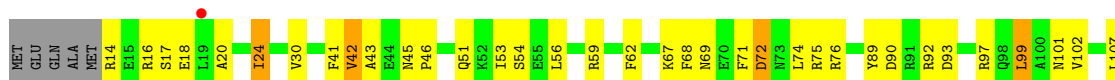
• Molecule 3: Proteasome subunit alpha



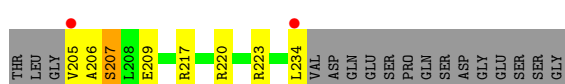
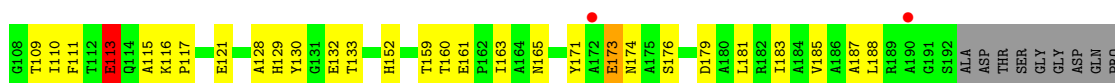
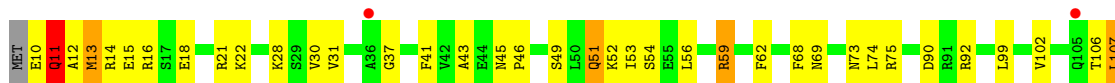
• Molecule 3: Proteasome subunit alpha



• Molecule 3: Proteasome subunit alpha



• Molecule 3: Proteasome subunit alpha



• Molecule 3: Proteasome subunit alpha



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	118.97Å 207.55Å 142.28Å 90.00° 102.42° 90.00°	Depositor
Resolution (Å)	29.87 – 2.60 29.87 – 2.60	Depositor EDS
% Data completeness (in resolution range)	96.5 (29.87-2.60) 96.4 (29.87-2.60)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.90 (at 2.57Å)	Xtrriage
Refinement program	CNS	Depositor
R, R_{free}	0.224 , 0.257 0.224 , 0.255	Depositor DCC
R_{free} test set	10154 reflections (4.74%)	wwPDB-VP
Wilson B-factor (Å ²)	38.0	Xtrriage
Anisotropy	0.235	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 46.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	46890	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.13% 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: OZT

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	2	0.93	2/1655 (0.1%)	1.08	4/2244 (0.2%)
1	C	0.88	0/1655	1.07	2/2244 (0.1%)
1	E	0.91	1/1655 (0.1%)	1.06	5/2244 (0.2%)
1	H	0.93	1/1655 (0.1%)	1.09	6/2244 (0.3%)
1	J	0.89	1/1655 (0.1%)	1.08	5/2244 (0.2%)
1	L	0.92	0/1655	1.09	3/2244 (0.1%)
1	N	1.06	2/1655 (0.1%)	1.10	5/2244 (0.2%)
1	P	1.05	2/1655 (0.1%)	1.08	4/2244 (0.2%)
1	R	0.90	0/1655	1.05	7/2244 (0.3%)
1	T	0.97	3/1655 (0.2%)	1.12	3/2244 (0.1%)
1	X	1.00	2/1655 (0.1%)	1.09	5/2244 (0.2%)
1	Z	0.89	1/1655 (0.1%)	1.11	3/2244 (0.1%)
2	G	0.88	2/1662 (0.1%)	1.12	6/2254 (0.3%)
2	V	1.03	2/1671 (0.1%)	1.05	3/2266 (0.1%)
3	1	0.83	0/1667	1.16	6/2251 (0.3%)
3	A	0.92	0/1675	1.12	11/2261 (0.5%)
3	B	0.94	0/1686	1.12	12/2276 (0.5%)
3	D	0.80	0/1667	1.11	7/2251 (0.3%)
3	F	0.89	1/1658 (0.1%)	1.22	15/2239 (0.7%)
3	I	0.90	1/1694 (0.1%)	1.09	9/2287 (0.4%)
3	K	0.82	1/1686 (0.1%)	1.13	12/2277 (0.5%)
3	M	0.78	0/1513	1.08	7/2048 (0.3%)
3	O	0.86	2/1674 (0.1%)	1.12	13/2261 (0.6%)
3	Q	0.78	1/1667 (0.1%)	1.18	11/2251 (0.5%)
3	S	0.86	1/1682 (0.1%)	1.12	10/2271 (0.4%)
3	U	0.80	0/1661	1.16	6/2243 (0.3%)
3	W	0.76	0/1636	1.02	3/2210 (0.1%)
3	Y	0.80	0/1667	1.07	8/2251 (0.4%)
All	All	0.90	26/46426 (0.1%)	1.10	191/62825 (0.3%)

The worst 5 of 26 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	314	MET	SD-CE	-9.35	1.56	1.79
1	P	314	MET	SD-CE	-9.24	1.56	1.79
2	G	361	VAL	C-N	-7.22	1.24	1.33
1	N	314	MET	SD-CE	-7.19	1.61	1.79
1	2	314	MET	SD-CE	-6.82	1.62	1.79

The worst 5 of 191 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	49	SER	N-CA-C	10.69	122.93	111.28
3	1	113	GLU	N-CA-C	9.51	121.41	111.14
3	I	49	SER	N-CA-C	9.43	121.64	111.36
3	B	113	GLU	N-CA-C	9.16	122.96	111.69
3	D	173	GLU	N-CA-C	9.12	122.37	111.33

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	2	1640	0	1630	32	0
1	C	1640	0	1630	42	0
1	E	1640	0	1630	31	0
1	H	1640	0	1630	31	0
1	J	1640	0	1630	23	0
1	L	1640	0	1630	39	0
1	N	1640	0	1630	38	0
1	P	1640	0	1630	37	0
1	R	1640	0	1630	39	0
1	T	1640	0	1630	40	0
1	X	1640	0	1630	33	0
1	Z	1640	0	1630	26	0
2	G	1638	0	1630	31	0
2	V	1647	0	1638	69	0
3	1	1643	0	1641	29	0
3	A	1651	0	1650	52	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	1662	0	1662	38	0
3	D	1643	0	1641	44	0
3	F	1634	0	1635	80	0
3	I	1670	0	1673	56	0
3	K	1662	0	1664	54	0
3	M	1489	0	1474	58	0
3	O	1650	0	1650	66	0
3	Q	1643	0	1641	78	0
3	S	1658	0	1659	57	0
3	U	1637	0	1636	76	0
3	W	1612	0	1613	44	0
3	Y	1643	0	1641	57	0
4	1	22	0	0	1	0
4	2	45	0	0	10	0
4	A	36	0	0	5	0
4	B	46	0	0	4	0
4	C	33	0	0	3	0
4	D	18	0	0	8	0
4	E	38	0	0	7	0
4	F	33	0	0	1	0
4	G	41	0	0	3	0
4	H	42	0	0	5	0
4	I	39	0	0	4	0
4	J	33	0	0	5	0
4	K	30	0	0	5	0
4	L	43	0	0	4	0
4	M	19	0	0	4	0
4	N	74	0	0	4	0
4	O	33	0	0	4	0
4	P	68	0	0	6	0
4	Q	13	0	0	2	0
4	R	41	0	0	6	0
4	S	19	0	0	0	0
4	T	34	0	0	2	0
4	U	31	0	0	9	0
4	V	70	0	0	4	0
4	W	18	0	0	0	0
4	X	51	0	0	3	0
4	Y	23	0	0	4	0
4	Z	35	0	0	2	0
All	All	46890	0	45708	1191	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 13.

The worst 5 of 1191 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)
1:2:301:OZT:H17	1:2:333:LYS:NZ	1.32	1.39
2:V:348:THR:HG22	2:V:351:VAL:CG2	1.58	1.33
3:Q:181:LEU:C	3:Q:181:LEU:HD12	1.55	1.29
3:U:163:ILE:CG1	3:U:191:GLY:HA3	1.65	1.27
1:C:349:ALA:O	1:C:353:VAL:HG22	1.38	1.24

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	2	220/240 (92%)	216 (98%)	4 (2%)	0	100	100
1	C	220/240 (92%)	218 (99%)	2 (1%)	0	100	100
1	E	220/240 (92%)	218 (99%)	2 (1%)	0	100	100
1	H	220/240 (92%)	216 (98%)	4 (2%)	0	100	100
1	J	220/240 (92%)	217 (99%)	3 (1%)	0	100	100
1	L	220/240 (92%)	218 (99%)	2 (1%)	0	100	100
1	N	220/240 (92%)	216 (98%)	4 (2%)	0	100	100
1	P	220/240 (92%)	218 (99%)	2 (1%)	0	100	100
1	R	220/240 (92%)	218 (99%)	1 (0%)	1 (0%)	24	46
1	T	220/240 (92%)	217 (99%)	3 (1%)	0	100	100
1	X	220/240 (92%)	217 (99%)	3 (1%)	0	100	100
1	Z	220/240 (92%)	217 (99%)	3 (1%)	0	100	100
2	G	220/240 (92%)	216 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	V	222/240 (92%)	219 (99%)	3 (1%)	0	100	100
3	1	209/240 (87%)	199 (95%)	9 (4%)	1 (0%)	24	46
3	A	210/240 (88%)	202 (96%)	8 (4%)	0	100	100
3	B	212/240 (88%)	205 (97%)	7 (3%)	0	100	100
3	D	209/240 (87%)	203 (97%)	6 (3%)	0	100	100
3	F	208/240 (87%)	203 (98%)	5 (2%)	0	100	100
3	I	213/240 (89%)	209 (98%)	4 (2%)	0	100	100
3	K	212/240 (88%)	206 (97%)	6 (3%)	0	100	100
3	M	190/240 (79%)	184 (97%)	6 (3%)	0	100	100
3	O	210/240 (88%)	204 (97%)	6 (3%)	0	100	100
3	Q	209/240 (87%)	202 (97%)	7 (3%)	0	100	100
3	S	211/240 (88%)	203 (96%)	8 (4%)	0	100	100
3	U	208/240 (87%)	201 (97%)	7 (3%)	0	100	100
3	W	205/240 (85%)	198 (97%)	7 (3%)	0	100	100
3	Y	209/240 (87%)	198 (95%)	11 (5%)	0	100	100
All	All	5997/6720 (89%)	5858 (98%)	137 (2%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	R	389	GLY
3	1	227	GLY

5.3.2 Protein sidechains [i](#)

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	2	164/177 (93%)	156 (95%)	8 (5%)	22	47
1	C	164/177 (93%)	149 (91%)	15 (9%)	9	19
1	E	164/177 (93%)	151 (92%)	13 (8%)	11	26

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	H	164/177 (93%)	152 (93%)	12 (7%)	13	29
1	J	164/177 (93%)	153 (93%)	11 (7%)	15	33
1	L	164/177 (93%)	152 (93%)	12 (7%)	13	29
1	N	164/177 (93%)	154 (94%)	10 (6%)	17	37
1	P	164/177 (93%)	154 (94%)	10 (6%)	17	37
1	R	164/177 (93%)	152 (93%)	12 (7%)	13	29
1	T	164/177 (93%)	155 (94%)	9 (6%)	19	41
1	X	164/177 (93%)	153 (93%)	11 (7%)	15	33
1	Z	164/177 (93%)	150 (92%)	14 (8%)	10	22
2	G	165/178 (93%)	155 (94%)	10 (6%)	17	37
2	V	165/178 (93%)	153 (93%)	12 (7%)	13	29
3	1	163/184 (89%)	151 (93%)	12 (7%)	13	29
3	A	164/184 (89%)	149 (91%)	15 (9%)	9	19
3	B	165/184 (90%)	154 (93%)	11 (7%)	15	33
3	D	163/184 (89%)	144 (88%)	19 (12%)	5	11
3	F	162/184 (88%)	139 (86%)	23 (14%)	3	6
3	I	166/184 (90%)	158 (95%)	8 (5%)	23	47
3	K	165/184 (90%)	151 (92%)	14 (8%)	10	22
3	M	148/184 (80%)	137 (93%)	11 (7%)	13	29
3	O	164/184 (89%)	156 (95%)	8 (5%)	22	47
3	Q	163/184 (89%)	147 (90%)	16 (10%)	7	17
3	S	165/184 (90%)	151 (92%)	14 (8%)	10	22
3	U	162/184 (88%)	149 (92%)	13 (8%)	11	25
3	W	160/184 (87%)	144 (90%)	16 (10%)	7	16
3	Y	163/184 (89%)	152 (93%)	11 (7%)	15	33
All	All	4571/5056 (90%)	4221 (92%)	350 (8%)	12	27

5 of 350 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	I	107	LEU
3	S	73	ASN
3	K	73	ASN

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Mol	Chain	Res	Type
3	O	59	ARG
3	U	74	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 81 such sidechains are listed below:

Mol	Chain	Res	Type
3	S	69	ASN
3	Y	11	GLN
3	S	114	GLN
3	U	129	HIS
3	Y	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](#)

12 non-standard protein/DNA/RNA residues 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
1	OZT	J	301	1	6,9,10	4.97	4 (66%)	9,12,14	6.14	7 (77%)
1	OZT	2	301	1	6,9,10	4.77	4 (66%)	9,12,14	5.63	6 (66%)
1	OZT	N	301	1	6,9,10	5.00	5 (83%)	9,12,14	5.63	6 (66%)
1	OZT	T	301	1	6,9,10	5.72	5 (83%)	9,12,14	5.52	7 (77%)
1	OZT	X	301	1	6,9,10	5.47	5 (83%)	9,12,14	5.82	7 (77%)
1	OZT	P	301	1	6,9,10	6.57	4 (66%)	9,12,14	6.27	7 (77%)
1	OZT	R	301	1	6,9,10	5.54	5 (83%)	9,12,14	5.96	6 (66%)
1	OZT	C	301	1	6,9,10	5.54	5 (83%)	9,12,14	5.95	6 (66%)
1	OZT	E	301	1	6,9,10	5.72	3 (50%)	9,12,14	5.82	7 (77%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	OZT	Z	301	1	6,9,10	6.10	5 (83%)	9,12,14	5.52	6 (66%)
1	OZT	H	301	1	6,9,10	5.66	5 (83%)	9,12,14	6.09	6 (66%)
1	OZT	L	301	1	6,9,10	5.56	5 (83%)	9,12,14	5.94	6 (66%)

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
1	OZT	J	301	1	-	1/1/14/16	0/1/1/1
1	OZT	2	301	1	-	1/1/14/16	0/1/1/1
1	OZT	N	301	1	-	0/1/14/16	0/1/1/1
1	OZT	T	301	1	-	0/1/14/16	0/1/1/1
1	OZT	X	301	1	-	0/1/14/16	0/1/1/1
1	OZT	P	301	1	-	1/1/14/16	0/1/1/1
1	OZT	R	301	1	-	1/1/14/16	0/1/1/1
1	OZT	C	301	1	-	1/1/14/16	0/1/1/1
1	OZT	E	301	1	-	1/1/14/16	0/1/1/1
1	OZT	Z	301	1	-	1/1/14/16	0/1/1/1
1	OZT	H	301	1	-	1/1/14/16	0/1/1/1
1	OZT	L	301	1	-	1/1/14/16	0/1/1/1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	P	301	OZT	O1-C5	13.18	1.54	1.36
1	Z	301	OZT	O1-C5	12.79	1.53	1.36
1	E	301	OZT	O1-C5	11.62	1.52	1.36
1	H	301	OZT	O1-C5	11.45	1.51	1.36
1	J	301	OZT	O1-C5	10.76	1.50	1.36

The worst 5 of 77 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	301	OZT	O1-C5-N	9.55	117.65	109.87
1	P	301	OZT	O1-C2-CA	9.29	112.17	103.72
1	R	301	OZT	O1-C5-N	8.72	116.97	109.87
1	C	301	OZT	O1-C5-N	8.71	116.97	109.87
1	L	301	OZT	O1-C5-N	8.67	116.94	109.87

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	H	301	OZT	O-C-CA-C2
1	C	301	OZT	O-C-CA-C2
1	E	301	OZT	O-C-CA-C2
1	J	301	OZT	O-C-CA-C2
1	L	301	OZT	O-C-CA-C2

There are no ring outliers.

12 monomers are involved in 65 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	J	301	OZT	4	0
1	2	301	OZT	6	0
1	N	301	OZT	2	0
1	T	301	OZT	6	0
1	X	301	OZT	7	0
1	P	301	OZT	7	0
1	R	301	OZT	5	0
1	C	301	OZT	6	0
1	E	301	OZT	5	0
1	Z	301	OZT	7	0
1	H	301	OZT	6	0
1	L	301	OZT	4	0

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

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	2	221/240 (92%)	-0.09	2 (0%) 81 78	14, 40, 80, 106	0
1	C	221/240 (92%)	0.05	4 (1%) 67 63	16, 46, 84, 106	0
1	E	221/240 (92%)	-0.02	3 (1%) 73 69	22, 45, 81, 114	0
1	H	221/240 (92%)	-0.17	5 (2%) 61 55	14, 37, 86, 102	0
1	J	221/240 (92%)	-0.00	5 (2%) 61 55	17, 45, 86, 111	0
1	L	221/240 (92%)	-0.25	2 (0%) 81 78	10, 37, 82, 110	0
1	N	221/240 (92%)	-0.30	9 (4%) 41 36	6, 28, 85, 120	0
1	P	221/240 (92%)	-0.27	7 (3%) 50 44	10, 29, 78, 109	0
1	R	221/240 (92%)	0.04	1 (0%) 87 85	21, 48, 89, 115	0
1	T	221/240 (92%)	0.05	6 (2%) 56 50	12, 42, 84, 120	0
1	X	221/240 (92%)	-0.02	5 (2%) 61 55	16, 38, 80, 116	0
1	Z	221/240 (92%)	0.07	3 (1%) 73 69	21, 48, 84, 111	0
2	G	222/240 (92%)	0.04	4 (1%) 67 63	11, 45, 79, 109	0
2	V	224/240 (93%)	-0.23	7 (3%) 51 45	9, 30, 79, 108	0
3	1	213/240 (88%)	0.69	16 (7%) 20 16	27, 70, 104, 115	0
3	A	214/240 (89%)	0.13	4 (1%) 66 61	7, 45, 85, 101	0
3	B	216/240 (90%)	0.18	9 (4%) 40 35	6, 40, 85, 102	0
3	D	213/240 (88%)	0.73	14 (6%) 24 19	19, 70, 102, 125	0
3	F	212/240 (88%)	0.46	16 (7%) 20 16	16, 55, 128, 161	0
3	I	217/240 (90%)	0.11	2 (0%) 81 78	15, 44, 83, 101	0
3	K	216/240 (90%)	0.38	4 (1%) 66 61	18, 60, 94, 115	0
3	M	194/240 (80%)	0.66	15 (7%) 19 15	26, 73, 103, 116	0
3	O	214/240 (89%)	0.32	8 (3%) 45 39	16, 55, 93, 106	0
3	Q	213/240 (88%)	0.85	20 (9%) 14 11	27, 70, 108, 130	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
3	S	215/240 (89%)	0.33	6 (2%) 55 49	17, 56, 95, 113	0
3	U	212/240 (88%)	1.17	43 (20%) 3 2	20, 76, 105, 120	0
3	W	209/240 (87%)	0.63	7 (3%) 49 43	25, 66, 99, 112	0
3	Y	213/240 (88%)	0.47	6 (2%) 55 49	19, 62, 97, 114	0
All	All	6069/6720 (90%)	0.21	233 (3%) 44 38	6, 49, 95, 161	0

The worst 5 of 233 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	V	349	ALA	5.5
1	P	353	VAL	4.8
1	H	349	ALA	4.7
3	W	205	VAL	4.5
1	X	425	ALA	4.4

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	OZT	Z	301	9/10	0.83	0.13	36,41,47,48	0
1	OZT	R	301	9/10	0.84	0.13	63,65,66,68	0
1	OZT	T	301	9/10	0.86	0.14	31,38,44,46	0
1	OZT	C	301	9/10	0.86	0.16	72,76,77,78	0
1	OZT	P	301	9/10	0.90	0.11	34,41,46,47	0
1	OZT	H	301	9/10	0.90	0.11	35,41,45,46	0
1	OZT	E	301	9/10	0.90	0.12	36,42,46,48	0
1	OZT	J	301	9/10	0.90	0.09	34,38,40,41	0
1	OZT	L	301	9/10	0.91	0.10	27,33,36,37	0
1	OZT	2	301	9/10	0.91	0.10	31,34,39,43	0
1	OZT	X	301	9/10	0.94	0.08	24,28,31,32	0
1	OZT	N	301	9/10	0.96	0.07	23,26,31,32	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.