



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 02:35 PM UTC

PDB ID : 3HFA / pdb_00003hfa
Title : Crystal Structure of Mycobacterium Tuberculosis Proteasome open-gate mutant
Authors : Li, D.; Li, H.
Deposited on : 2009-05-11
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

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

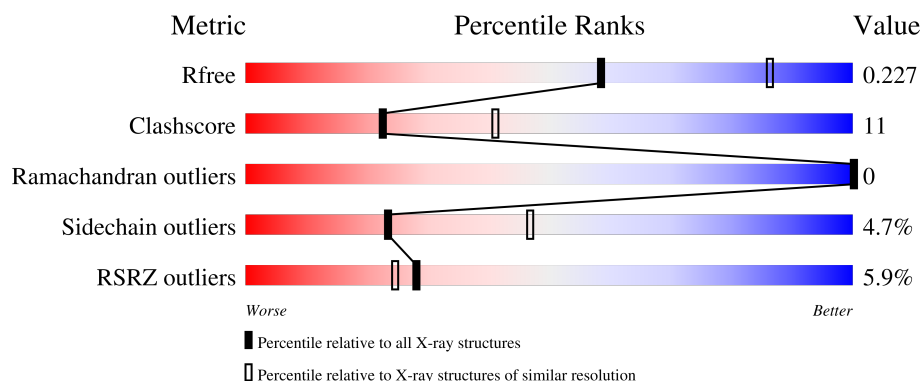
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (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 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	% 82% 10% 8%
1	C	240	3% 82% 10% 8%
1	E	240	% 79% 13% 7%
1	G	240	81% 10% 8%
1	H	240	% 83% 9% 7%

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Mol	Chain	Length	Quality of chain
1	J	240	
1	L	240	
1	N	240	
1	P	240	
1	R	240	
1	T	240	
1	V	240	
1	X	240	
1	Z	240	
2	1	240	
2	A	240	
2	B	240	
2	D	240	
2	F	240	
2	I	240	
2	K	240	
2	M	240	
2	O	240	
2	Q	240	
2	S	240	
2	U	240	
2	W	240	
2	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
3	DMF	K	251	-	-	X	-
3	DMF	Q	251	-	-	X	-
3	DMF	Z	69	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 48523 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 (Beta subunit) PrcB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	223	Total	C	N	O	S	0	0	0
			1642	1029	283	325	5			
1	C	222	Total	C	N	O	S	0	0	0
			1638	1027	282	324	5			
1	E	223	Total	C	N	O	S	0	0	0
			1642	1029	283	325	5			
1	G	222	Total	C	N	O	S	0	0	0
			1638	1027	282	324	5			
1	J	222	Total	C	N	O	S	0	0	0
			1638	1027	282	324	5			
1	L	222	Total	C	N	O	S	0	0	0
			1638	1027	282	324	5			
1	N	223	Total	C	N	O	S	0	0	0
			1642	1029	283	325	5			
1	P	222	Total	C	N	O	S	0	0	0
			1638	1027	282	324	5			
1	R	222	Total	C	N	O	S	0	0	0
			1638	1027	282	324	5			
1	T	223	Total	C	N	O	S	0	0	0
			1642	1029	283	325	5			
1	V	226	Total	C	N	O	S	0	0	0
			1662	1040	286	331	5			
1	X	224	Total	C	N	O	S	0	0	0
			1647	1032	284	326	5			
1	Z	224	Total	C	N	O	S	0	0	0
			1647	1032	284	326	5			
1	2	222	Total	C	N	O	S	0	0	0
			1638	1027	282	324	5			

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	535	HIS	-	expression tag	UNP O33245

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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 2 is a protein called Proteasome (Alpha subunit) PrcA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	213	Total 1645	C 1030	N 301	O 310	S 4	0	0	0
2	A	214	Total 1653	C 1036	N 302	O 311	S 4	0	0	0
2	B	214	Total 1653	C 1036	N 302	O 311	S 4	0	0	0
2	F	214	Total 1653	C 1036	N 302	O 311	S 4	0	0	0
2	I	214	Total 1653	C 1036	N 302	O 311	S 4	0	0	0
2	K	214	Total 1653	C 1036	N 302	O 311	S 4	0	0	0
2	M	214	Total 1653	C 1036	N 302	O 311	S 4	0	0	0
2	O	214	Total 1653	C 1036	N 302	O 311	S 4	0	0	0
2	Q	214	Total 1653	C 1036	N 302	O 311	S 4	0	0	0
2	S	214	Total 1653	C 1036	N 302	O 311	S 4	0	0	0
2	U	214	Total 1653	C 1036	N 302	O 311	S 4	0	0	0
2	W	214	Total 1653	C 1036	N 302	O 311	S 4	0	0	0
2	Y	214	Total 1653	C 1036	N 302	O 311	S 4	0	0	0
2	1	214	Total 1653	C 1036	N 302	O 311	S 4	0	0	0

There are 14 discrepancies between the modelled and reference sequences:

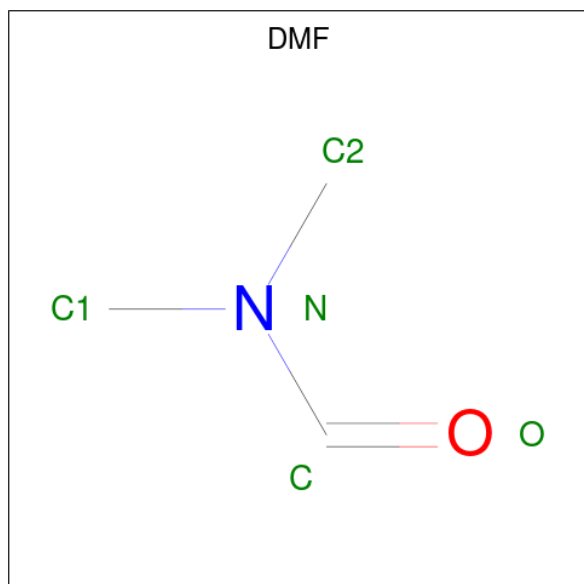
Chain	Residue	Modelled	Actual	Comment	Reference
D	9	MET	-	initiating methionine	UNP O33244
A	9	MET	-	initiating methionine	UNP O33244
B	9	MET	-	initiating methionine	UNP O33244
F	9	MET	-	initiating methionine	UNP O33244
I	9	MET	-	initiating methionine	UNP O33244
K	9	MET	-	initiating methionine	UNP O33244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

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Chain	Residue	Modelled	Actual	Comment	Reference
Y	9	MET	-	initiating methionine	UNP O33244
1	9	MET	-	initiating methionine	UNP O33244

- Molecule 3 is DIMETHYLFORMAMIDE (CCD ID: DMF) (formula: C_3H_7NO).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	H	1	Total	C	N	O	0	0
			5	3	1	1		
3	H	1	Total	C	N	O	0	0
			5	3	1	1		
3	C	1	Total	C	N	O	0	0
			5	3	1	1		
3	E	1	Total	C	N	O	0	0
			5	3	1	1		
3	E	1	Total	C	N	O	0	0
			5	3	1	1		
3	E	1	Total	C	N	O	0	0
			5	3	1	1		
3	G	1	Total	C	N	O	0	0
			5	3	1	1		
3	G	1	Total	C	N	O	0	0
			5	3	1	1		
3	G	1	Total	C	N	O	0	0
			5	3	1	1		
3	J	1	Total	C	N	O	0	0
			5	3	1	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	L	1	Total	C	N	O	0	0
			5	3	1	1		
3	L	1	Total	C	N	O	0	0
			5	3	1	1		
3	L	1	Total	C	N	O	0	0
			5	3	1	1		
3	L	1	Total	C	N	O	0	0
			5	3	1	1		
3	N	1	Total	C	N	O	0	0
			5	3	1	1		
3	N	1	Total	C	N	O	0	0
			5	3	1	1		
3	P	1	Total	C	N	O	0	0
			5	3	1	1		
3	P	1	Total	C	N	O	0	0
			5	3	1	1		
3	P	1	Total	C	N	O	0	0
			5	3	1	1		
3	T	1	Total	C	N	O	0	0
			5	3	1	1		
3	T	1	Total	C	N	O	0	0
			5	3	1	1		
3	V	1	Total	C	N	O	0	0
			5	3	1	1		
3	V	1	Total	C	N	O	0	0
			5	3	1	1		
3	V	1	Total	C	N	O	0	0
			5	3	1	1		
3	V	1	Total	C	N	O	0	0
			5	3	1	1		
3	V	1	Total	C	N	O	0	0
			5	3	1	1		
3	X	1	Total	C	N	O	0	0
			5	3	1	1		
3	Z	1	Total	C	N	O	0	0
			5	3	1	1		
3	Z	1	Total	C	N	O	0	0
			5	3	1	1		
3	Z	1	Total	C	N	O	0	0
			5	3	1	1		
3	Z	1	Total	C	N	O	0	0
			5	3	1	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	Z	1	Total 5	C 3	N 1	O 1	0	0
3	2	1	Total 5	C 3	N 1	O 1	0	0
3	2	1	Total 5	C 3	N 1	O 1	0	0
3	D	1	Total 5	C 3	N 1	O 1	0	0
3	A	1	Total 5	C 3	N 1	O 1	0	0
3	A	1	Total 5	C 3	N 1	O 1	0	0
3	B	1	Total 5	C 3	N 1	O 1	0	0
3	F	1	Total 5	C 3	N 1	O 1	0	0
3	I	1	Total 5	C 3	N 1	O 1	0	0
3	K	1	Total 5	C 3	N 1	O 1	0	0
3	K	1	Total 5	C 3	N 1	O 1	0	0
3	K	1	Total 5	C 3	N 1	O 1	0	0
3	M	1	Total 5	C 3	N 1	O 1	0	0
3	O	1	Total 5	C 3	N 1	O 1	0	0
3	Q	1	Total 5	C 3	N 1	O 1	0	0
3	Q	1	Total 5	C 3	N 1	O 1	0	0
3	Q	1	Total 5	C 3	N 1	O 1	0	0
3	S	1	Total 5	C 3	N 1	O 1	0	0
3	S	1	Total 5	C 3	N 1	O 1	0	0
3	U	1	Total 5	C 3	N 1	O 1	0	0
3	U	1	Total 5	C 3	N 1	O 1	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	W	1	Total	C	N	O	0	0
			5	3	1	1		
3	Y	1	Total	C	N	O	0	0
			5	3	1	1		
3	Y	1	Total	C	N	O	0	0
			5	3	1	1		
3	Y	1	Total	C	N	O	0	0
			5	3	1	1		
3	1	1	Total	C	N	O	0	0
			5	3	1	1		
3	1	1	Total	C	N	O	0	0
			5	3	1	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	H	92	Total	O	0	0
			92	92		
4	C	43	Total	O	0	0
			43	43		
4	E	121	Total	O	0	0
			121	121		
4	G	113	Total	O	0	0
			113	113		
4	J	73	Total	O	0	0
			73	73		
4	L	109	Total	O	0	0
			109	109		
4	N	124	Total	O	0	0
			124	124		
4	P	93	Total	O	0	0
			93	93		
4	R	89	Total	O	0	0
			89	89		
4	T	96	Total	O	0	0
			96	96		
4	V	133	Total	O	0	0
			133	133		
4	X	101	Total	O	0	0
			101	101		
4	Z	91	Total	O	0	0
			91	91		

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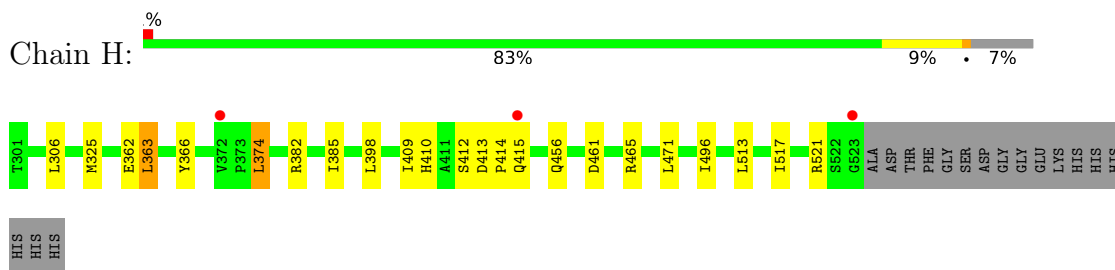
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	2	107	Total 107	O 107	0	0
4	D	49	Total 49	O 49	0	0
4	A	31	Total 31	O 31	0	0
4	B	37	Total 37	O 37	0	0
4	F	60	Total 60	O 60	0	0
4	I	35	Total 35	O 35	0	0
4	K	52	Total 52	O 52	0	0
4	M	74	Total 74	O 74	0	0
4	O	34	Total 34	O 34	0	0
4	Q	71	Total 71	O 71	0	0
4	S	35	Total 35	O 35	0	0
4	U	48	Total 48	O 48	0	0
4	W	62	Total 62	O 62	0	0
4	Y	68	Total 68	O 68	0	0
4	1	68	Total 68	O 68	0	0

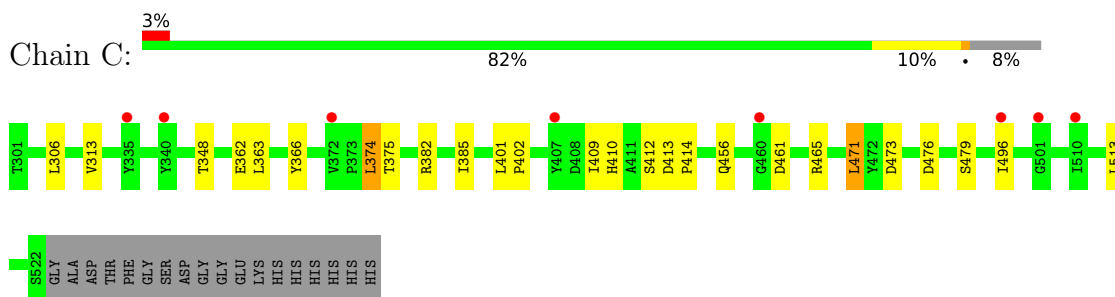
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

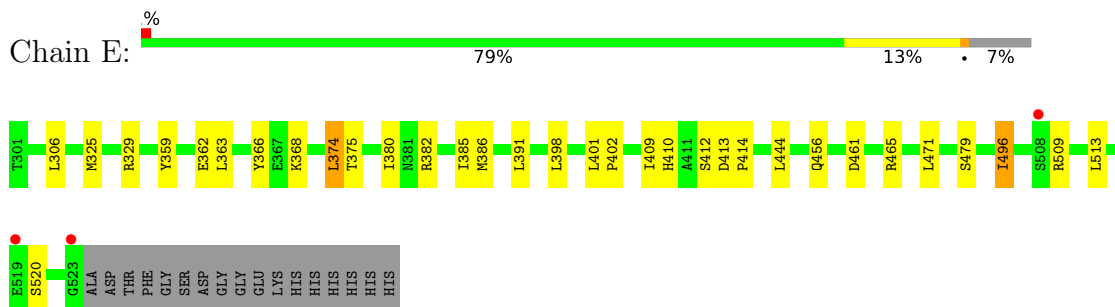
- Molecule 1: Proteasome (Beta subunit) PrcB



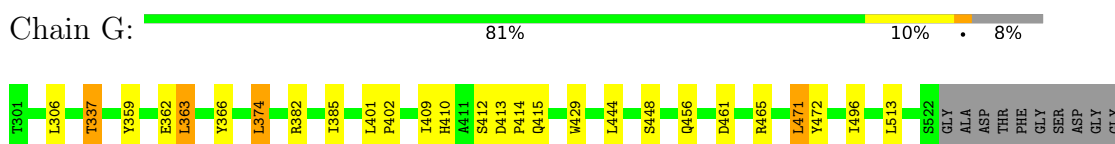
- Molecule 1: Proteasome (Beta subunit) PrcB



- Molecule 1: Proteasome (Beta subunit) PrcB



- Molecule 1: Proteasome (Beta subunit) PrcB



GLU
LYS
HIS
HIS
HIS
HIS
HIS
HIS

• Molecule 1: Proteasome (Beta subunit) PrcB

Chain J:  2% 83% 8% 8%

T301 L306 E362 L363 Y366 E367 K368 L374 R382 I385 L391 I409 H410 A411 S412 D413 P414 L444 Q456 D461 R465 L471 I496 L513 A514 R515 I518 E519 S522 GLY ALA ASP THR PHE GLY SER ASP GLY GLU LYS HIS HIS

HIS
HIS
HIS
HIS

• Molecule 1: Proteasome (Beta subunit) PrcB

Chain L:  81% 11% 8%

T301 L306 M325 D339 E362 L363 Y366 L374 T375 R382 K379 R382 I385 L391 L398 I409 H410 A411 S412 D413 P414 Q415 S416 L444 Q456 R465 L471 G482 G483 I496 L513 S522 GLY ALA ASP THR PHE GLY SER ASP GLY

GLY
GLU
LYS
HIS
HIS
HIS
HIS
HIS

• Molecule 1: Proteasome (Beta subunit) PrcB

Chain N:  82% 10% 7%

T301 L306 R332 E362 L363 Y366 L374 T375 R382 I385 R388 L398 I409 H410 A411 S412 D413 P414 W429 Q456 D461 R465 D473 I496 D500 L513 E519 S520 R521 S522 G523 ALA ASP THR PHE GLY SER ASP GLY GLU

LYS
HIS
HIS
HIS
HIS
HIS
HIS

• Molecule 1: Proteasome (Beta subunit) PrcB

Chain P:  83% 8% 8%

T301 L306 E362 L363 Y366 L374 A377 N381 R382 I385 L391 Q396 I409 H410 A411 S412 D413 P414 L444 Q456 D461 R465 L471 I496 L513 S522 GLY ALA ASP THR PHE GLY SER ASP GLY GLU LYS HIS HIS HIS

HIS
HIS

• Molecule 1: Proteasome (Beta subunit) PrcB

Chain R:  81% 11% 8%

T301 L306 E362 L363 Y366 L374 R382 I385 L391 L401 P402 I409 H410 A411 S412 D413 P414 W429 E432 F433 E434 L444 K451 K452 Q456 D461 R465 L471 I496 R509 L513 A514 R515 S522 GLY ALA ASP THR PHE

GLY
SER
ASP
GLY
GLY
GLY
LYS
HIS
HIS
HIS
HIS
HIS

• Molecule 1: Proteasome (Beta subunit) PrcB

Chain T:  82% 10% 7%

T301 L306 E362 L363 Y366 L374 A377 R382 I385 L391 M395 L398 I409 H410 A411 S412 D413 P414 L444 Q456 D461 R465 L471 Y472 I496 L513 S522 G523 ALA ASP THR PHE GLY SER ASP GLY GLY LYS HIS

HIS
HIS
HIS
HIS

• Molecule 1: Proteasome (Beta subunit) PrcB

Chain V:  82% 10% 6%

T301 L306 R319 I345 R357 E362 L363 Y366 L374 T375 R382 I385 R388 I409 H410 A411 S412 D413 P414 W429 K451 Q456 D461 R465 L471 I496 L513 A514 R515 S522 G523 T526 PHE GLY SER ASP GLY GLU

LYS
HIS
HIS
HIS
HIS
HIS
HIS

• Molecule 1: Proteasome (Beta subunit) PrcB

Chain X:  84% 9% 7%

T301 L306 M325 E362 L363 Y366 L374 R382 I385 L391 Q396 I409 A411 S412 D413 P414 K451 Q456 D461 R465 L471 I496 L513 S522 G523 A524 ASP THR PHE GLY SER ASP GLY GLY LYS HIS HIS HIS HIS

HIS

• Molecule 1: Proteasome (Beta subunit) PrcB

Chain Z:  83% 9% 7%

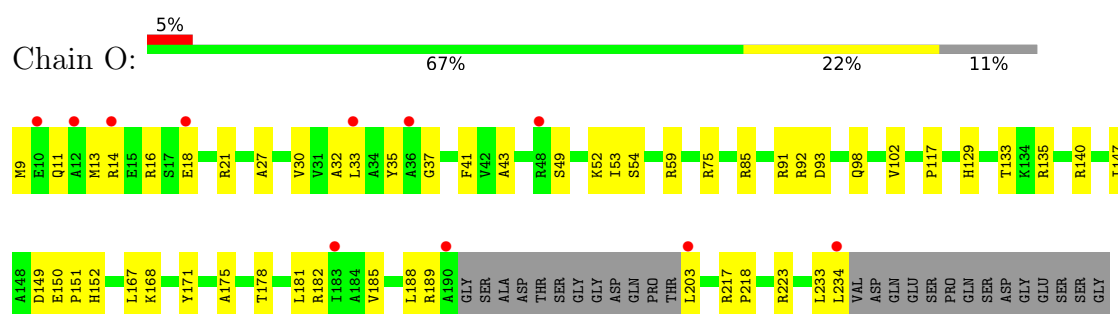
T301 L306 R357 E362 L363 Y366 L374 R382 I385 L398 I409 H410 A411 S412 D413 P414 W429 L444 Q456 D461 R465 L471 I496 R509 L513 S522 G523 A524 ASP THR PHE GLY SER ASP GLY GLY LYS HIS HIS HIS

HIS
HIS
HIS

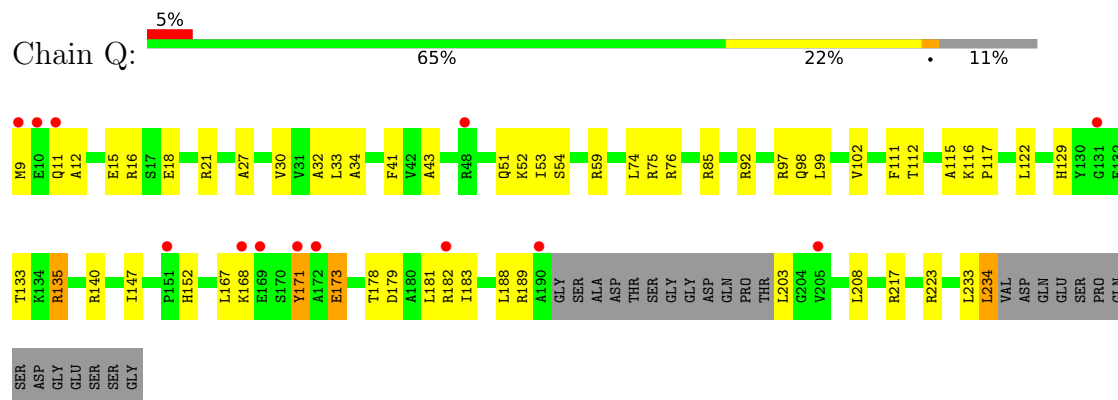
• Molecule 1: Proteasome (Beta subunit) PrcB

Chain 2:  82% 10% 8%

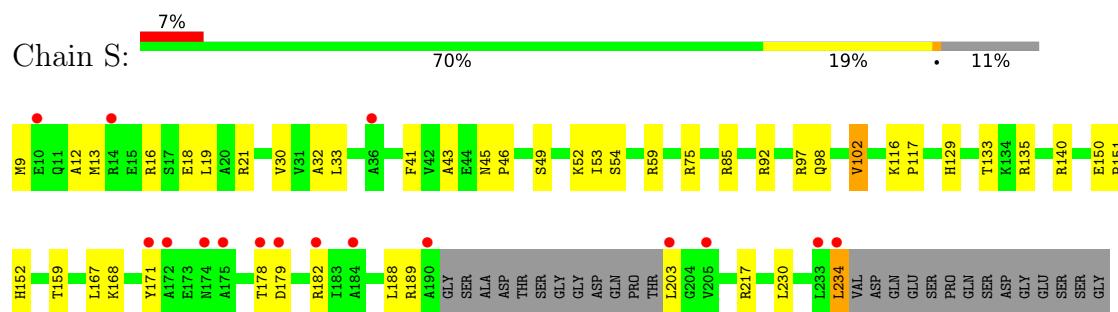
T301 L306 M325 E362 L363 Y366 L374 R382 I385 Q396 G397 L398 L401 P402 I409 H410 A411 S412 D413 P414 W429 L444 S448 D461 L471 Y472 I496 L513 E519 S522 G523 GLY ALA ASP THR PHE GLY SER ASP GLY GLY LYS HIS HIS HIS



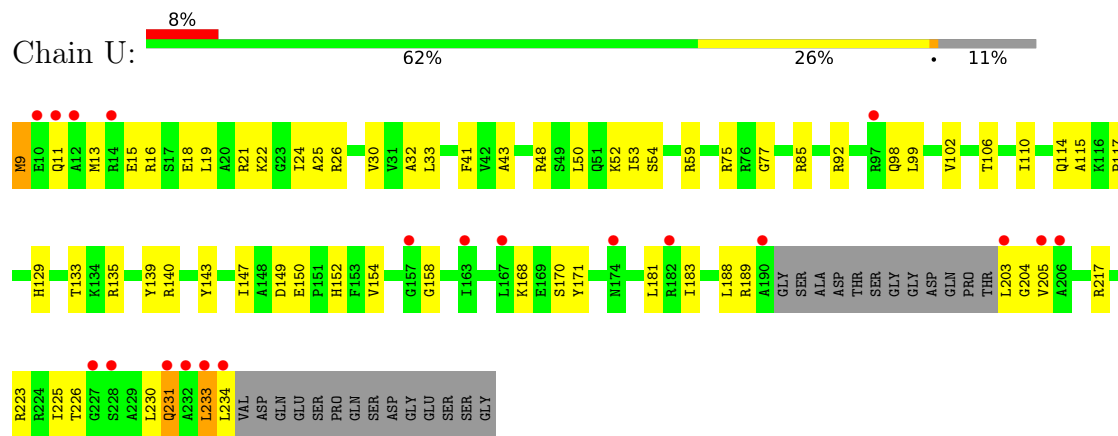
• Molecule 2: Proteasome (Alpha subunit) PrcA



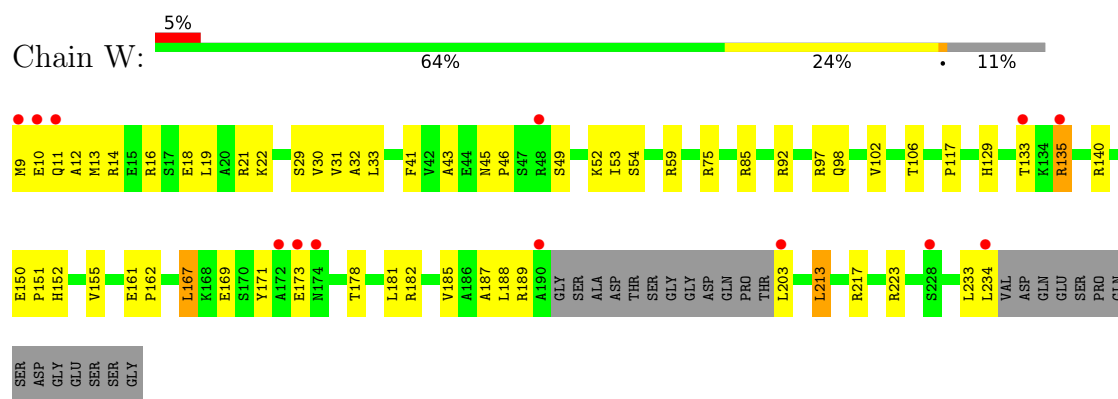
• Molecule 2: Proteasome (Alpha subunit) PrcA



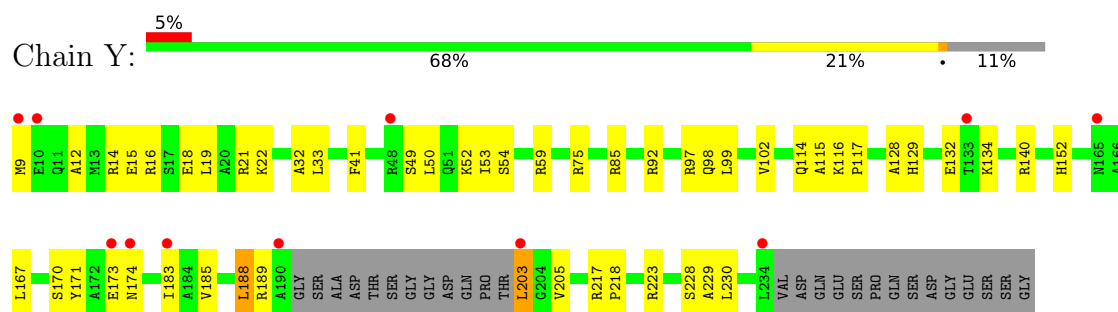
• Molecule 2: Proteasome (Alpha subunit) PrcA



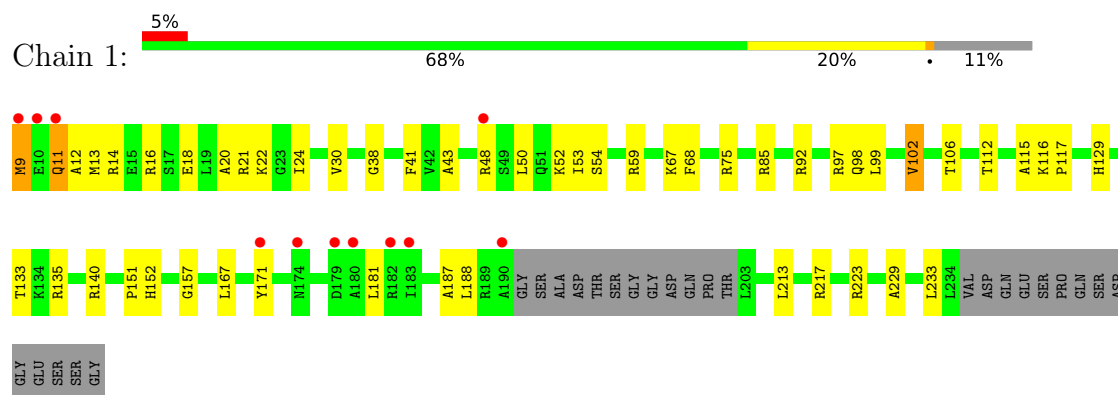
• Molecule 2: Proteasome (Alpha subunit) PrcA



• Molecule 2: Proteasome (Alpha subunit) PrcA



• Molecule 2: Proteasome (Alpha subunit) PrcA



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	119.16Å 221.44Å 137.12Å 90.00° 104.89° 90.00°	Depositor
Resolution (Å)	29.86 – 2.50 29.86 – 2.50	Depositor EDS
% Data completeness (in resolution range)	97.8 (29.86-2.50) 97.7 (29.86-2.50)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.80 (at 2.51Å)	Xtriage
Refinement program	PHENIX (phenix.refine), CNS	Depositor
R, R_{free}	0.173 , 0.214 0.199 , 0.227	Depositor DCC
R_{free} test set	11458 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å ²)	33.3	Xtriage
Anisotropy	0.164	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 54.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	48523	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.15% 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 ⓘ

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

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	0.46	0/1662	0.72	2/2254 (0.1%)
1	C	0.41	0/1662	0.73	2/2254 (0.1%)
1	E	0.45	0/1666	0.72	2/2259 (0.1%)
1	G	0.50	0/1662	0.75	2/2254 (0.1%)
1	H	0.44	0/1666	0.72	2/2259 (0.1%)
1	J	0.41	0/1662	0.70	2/2254 (0.1%)
1	L	0.45	0/1662	0.72	2/2254 (0.1%)
1	N	0.48	0/1666	0.73	3/2259 (0.1%)
1	P	0.45	0/1662	0.71	2/2254 (0.1%)
1	R	0.43	0/1662	0.72	2/2254 (0.1%)
1	T	0.44	0/1666	0.72	3/2259 (0.1%)
1	V	0.48	0/1686	0.77	4/2287 (0.2%)
1	X	0.43	0/1671	0.72	3/2266 (0.1%)
1	Z	0.43	0/1671	0.71	3/2266 (0.1%)
2	1	0.43	0/1677	0.77	0/2264
2	A	0.39	0/1677	0.76	0/2264
2	B	0.43	0/1677	0.92	6/2264 (0.3%)
2	D	0.48	1/1669 (0.1%)	0.81	2/2253 (0.1%)
2	F	0.40	0/1677	0.76	0/2264
2	I	0.42	0/1677	0.81	1/2264 (0.0%)
2	K	0.40	0/1677	0.76	0/2264
2	M	0.42	0/1677	0.79	2/2264 (0.1%)
2	O	0.40	0/1677	0.74	0/2264
2	Q	0.46	0/1677	0.80	3/2264 (0.1%)
2	S	0.38	0/1677	0.74	0/2264
2	U	0.43	0/1677	0.78	0/2264
2	W	0.42	0/1677	0.79	3/2264 (0.1%)
2	Y	0.44	0/1677	0.78	0/2264
All	All	0.44	1/46796 (0.0%)	0.76	51/63318 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	9	MET	C-N	-8.44	1.23	1.33

The worst 5 of 51 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	49	SER	N-CA-C	7.97	123.01	113.28
1	T	522	SER	N-CA-C	-7.65	102.88	111.14
1	V	523	GLY	N-CA-C	-7.45	104.27	115.00
2	D	228	SER	N-CA-C	7.20	120.04	111.33
1	N	522	SER	N-CA-C	6.71	119.87	109.60

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	1638	0	1630	17	0
1	C	1638	0	1630	23	0
1	E	1642	0	1633	31	0
1	G	1638	0	1630	22	0
1	H	1642	0	1633	16	0
1	J	1638	0	1630	15	0
1	L	1638	0	1630	22	0
1	N	1642	0	1633	20	0
1	P	1638	0	1630	19	0
1	R	1638	0	1630	23	0
1	T	1642	0	1633	20	0
1	V	1662	0	1649	23	0
1	X	1647	0	1638	17	0
1	Z	1647	0	1638	23	0
2	1	1653	0	1656	50	0
2	A	1653	0	1656	41	0
2	B	1653	0	1656	164	0
2	D	1645	0	1645	52	0
2	F	1653	0	1656	43	0
2	I	1653	0	1656	64	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	K	1653	0	1656	36	0
2	M	1653	0	1656	38	0
2	O	1653	0	1656	48	0
2	Q	1653	0	1656	43	0
2	S	1653	0	1656	51	0
2	U	1653	0	1656	51	0
2	W	1653	0	1656	56	0
2	Y	1653	0	1656	48	0
3	1	10	0	14	2	0
3	2	10	0	14	2	0
3	A	10	0	14	1	0
3	B	5	0	7	0	0
3	C	5	0	7	0	0
3	D	5	0	7	0	0
3	E	15	0	21	4	0
3	F	5	0	7	0	0
3	G	15	0	21	4	0
3	H	10	0	14	1	0
3	I	5	0	7	1	0
3	J	5	0	7	0	0
3	K	15	0	21	5	0
3	L	20	0	28	4	0
3	M	5	0	7	0	0
3	N	10	0	14	1	0
3	O	5	0	7	0	0
3	P	15	0	21	3	0
3	Q	15	0	21	5	0
3	S	10	0	14	1	0
3	T	10	0	14	5	0
3	U	10	0	14	1	0
3	V	25	0	35	7	0
3	W	5	0	7	1	0
3	X	5	0	7	0	0
3	Y	15	0	21	1	0
3	Z	25	0	35	7	0
4	1	68	0	0	1	0
4	2	107	0	0	3	0
4	A	31	0	0	0	0
4	B	37	0	0	4	0
4	C	43	0	0	1	0
4	D	49	0	0	5	0
4	E	121	0	0	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	F	60	0	0	4	0
4	G	113	0	0	2	0
4	H	92	0	0	0	0
4	I	35	0	0	6	0
4	J	73	0	0	2	0
4	K	52	0	0	3	0
4	L	109	0	0	4	0
4	M	74	0	0	5	0
4	N	124	0	0	6	0
4	O	34	0	0	4	0
4	P	93	0	0	2	0
4	Q	71	0	0	2	0
4	R	89	0	0	2	0
4	S	35	0	0	3	0
4	T	96	0	0	1	0
4	U	48	0	0	2	0
4	V	133	0	0	2	0
4	W	62	0	0	4	0
4	X	101	0	0	1	0
4	Y	68	0	0	3	0
4	Z	91	0	0	3	0
All	All	48523	0	46446	978	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 11.

The worst 5 of 978 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:O:9:MET:HE2	2:O:13:MET:CE	1.64	1.26
2:A:115:ALA:HB3	2:B:112:THR:CG2	1.66	1.25
2:S:116:LYS:HB2	2:1:13:MET:CE	1.68	1.23
2:S:230:LEU:O	2:S:234:LEU:HD13	1.34	1.22
2:B:9:MET:CE	2:B:13:MET:HE3	1.72	1.19

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	2	220/240 (92%)	218 (99%)	2 (1%)	0	100	100
1	C	220/240 (92%)	220 (100%)	0	0	100	100
1	E	221/240 (92%)	219 (99%)	2 (1%)	0	100	100
1	G	220/240 (92%)	218 (99%)	2 (1%)	0	100	100
1	H	221/240 (92%)	219 (99%)	2 (1%)	0	100	100
1	J	220/240 (92%)	219 (100%)	1 (0%)	0	100	100
1	L	220/240 (92%)	218 (99%)	2 (1%)	0	100	100
1	N	221/240 (92%)	218 (99%)	3 (1%)	0	100	100
1	P	220/240 (92%)	218 (99%)	2 (1%)	0	100	100
1	R	220/240 (92%)	218 (99%)	2 (1%)	0	100	100
1	T	221/240 (92%)	219 (99%)	2 (1%)	0	100	100
1	V	224/240 (93%)	222 (99%)	2 (1%)	0	100	100
1	X	222/240 (92%)	220 (99%)	2 (1%)	0	100	100
1	Z	222/240 (92%)	221 (100%)	1 (0%)	0	100	100
2	1	210/240 (88%)	206 (98%)	4 (2%)	0	100	100
2	A	210/240 (88%)	206 (98%)	4 (2%)	0	100	100
2	B	210/240 (88%)	201 (96%)	9 (4%)	0	100	100
2	D	209/240 (87%)	205 (98%)	4 (2%)	0	100	100
2	F	210/240 (88%)	206 (98%)	4 (2%)	0	100	100
2	I	210/240 (88%)	206 (98%)	4 (2%)	0	100	100
2	K	210/240 (88%)	206 (98%)	4 (2%)	0	100	100
2	M	210/240 (88%)	206 (98%)	4 (2%)	0	100	100
2	O	210/240 (88%)	205 (98%)	5 (2%)	0	100	100
2	Q	210/240 (88%)	206 (98%)	4 (2%)	0	100	100
2	S	210/240 (88%)	204 (97%)	6 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	U	210/240 (88%)	205 (98%)	5 (2%)	0	100	100
2	W	210/240 (88%)	207 (99%)	3 (1%)	0	100	100
2	Y	210/240 (88%)	205 (98%)	5 (2%)	0	100	100
All	All	6031/6720 (90%)	5941 (98%)	90 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	2	165/178 (93%)	158 (96%)	7 (4%)	26	52
1	C	165/178 (93%)	159 (96%)	6 (4%)	31	58
1	E	165/178 (93%)	159 (96%)	6 (4%)	31	58
1	G	165/178 (93%)	158 (96%)	7 (4%)	26	52
1	H	165/178 (93%)	159 (96%)	6 (4%)	31	58
1	J	165/178 (93%)	158 (96%)	7 (4%)	26	52
1	L	165/178 (93%)	160 (97%)	5 (3%)	36	64
1	N	165/178 (93%)	160 (97%)	5 (3%)	36	64
1	P	165/178 (93%)	159 (96%)	6 (4%)	31	58
1	R	165/178 (93%)	160 (97%)	5 (3%)	36	64
1	T	165/178 (93%)	159 (96%)	6 (4%)	31	58
1	V	167/178 (94%)	160 (96%)	7 (4%)	26	52
1	X	165/178 (93%)	159 (96%)	6 (4%)	31	58
1	Z	165/178 (93%)	159 (96%)	6 (4%)	31	58
2	1	164/184 (89%)	154 (94%)	10 (6%)	17	35
2	A	164/184 (89%)	153 (93%)	11 (7%)	15	31
2	B	164/184 (89%)	152 (93%)	12 (7%)	13	27
2	D	163/184 (89%)	156 (96%)	7 (4%)	26	51

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	F	164/184 (89%)	154 (94%)	10 (6%)	17	35
2	I	164/184 (89%)	155 (94%)	9 (6%)	19	40
2	K	164/184 (89%)	156 (95%)	8 (5%)	22	45
2	M	164/184 (89%)	153 (93%)	11 (7%)	15	31
2	O	164/184 (89%)	156 (95%)	8 (5%)	22	45
2	Q	164/184 (89%)	155 (94%)	9 (6%)	19	40
2	S	164/184 (89%)	156 (95%)	8 (5%)	22	45
2	U	164/184 (89%)	152 (93%)	12 (7%)	13	27
2	W	164/184 (89%)	155 (94%)	9 (6%)	19	40
2	Y	164/184 (89%)	157 (96%)	7 (4%)	26	51
All	All	4607/5068 (91%)	4391 (95%)	216 (5%)	23	47

5 of 216 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	F	52	LYS
2	M	52	LYS
2	Y	52	LYS
2	F	135	ARG
2	I	167	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 74 such sidechains are listed below:

Mol	Chain	Res	Type
2	S	98	GLN
2	1	98	GLN
2	U	69	ASN
2	W	129	HIS
1	Z	396	GLN

5.3.3 RNA ⓘ

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](#)

58 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	DMF	L	9	-	4,4,4	0.38	0	4,4,4	0.48	0
3	DMF	Z	105	-	4,4,4	0.39	0	4,4,4	0.39	0
3	DMF	M	249	-	4,4,4	0.39	0	4,4,4	0.38	0
3	DMF	S	250	-	4,4,4	0.37	0	4,4,4	0.36	0
3	DMF	X	141	-	4,4,4	0.31	0	4,4,4	0.36	0
3	DMF	2	145	-	4,4,4	0.32	0	4,4,4	0.44	0
3	DMF	K	251	-	4,4,4	0.36	0	4,4,4	0.28	0
3	DMF	A	8	-	4,4,4	0.26	0	4,4,4	0.29	0
3	DMF	V	16	-	4,4,4	0.36	0	4,4,4	0.41	0
3	DMF	Q	250	-	4,4,4	0.36	0	4,4,4	0.28	0
3	DMF	K	250	-	4,4,4	0.39	0	4,4,4	0.45	0
3	DMF	V	136	-	4,4,4	0.41	0	4,4,4	0.48	0
3	DMF	Z	27	-	4,4,4	0.35	0	4,4,4	0.46	0
3	DMF	C	15	-	4,4,4	0.33	0	4,4,4	0.41	0
3	DMF	P	23	-	4,4,4	0.33	0	4,4,4	0.42	0
3	DMF	Q	251	-	4,4,4	0.32	0	4,4,4	0.45	0
3	DMF	L	138	-	4,4,4	0.37	0	4,4,4	0.30	0
3	DMF	I	249	-	4,4,4	0.32	0	4,4,4	0.44	0
3	DMF	U	250	-	4,4,4	0.32	0	4,4,4	0.32	0
3	DMF	N	36	-	4,4,4	0.37	0	4,4,4	0.42	0
3	DMF	L	14	-	4,4,4	0.37	0	4,4,4	0.34	0
3	DMF	U	249	-	4,4,4	0.34	0	4,4,4	0.34	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	DMF	A	249	-	4,4,4	0.40	0	4,4,4	0.51	0
3	DMF	E	28	-	4,4,4	0.37	0	4,4,4	0.40	0
3	DMF	Z	50	-	4,4,4	0.35	0	4,4,4	0.41	0
3	DMF	Z	122	-	4,4,4	0.35	0	4,4,4	0.39	0
3	DMF	L	60	-	4,4,4	0.34	0	4,4,4	0.46	0
3	DMF	Y	249	-	4,4,4	0.49	0	4,4,4	0.58	0
3	DMF	1	249	-	4,4,4	0.39	0	4,4,4	0.27	0
3	DMF	W	249	-	4,4,4	0.30	0	4,4,4	0.22	0
3	DMF	E	104	-	4,4,4	0.29	0	4,4,4	0.45	0
3	DMF	J	46	-	4,4,4	0.38	0	4,4,4	0.52	0
3	DMF	V	117	-	4,4,4	0.40	0	4,4,4	0.44	0
3	DMF	G	20	-	4,4,4	0.37	0	4,4,4	0.25	0
3	DMF	2	99	-	4,4,4	0.36	0	4,4,4	0.46	0
3	DMF	S	249	-	4,4,4	0.32	0	4,4,4	0.31	0
3	DMF	V	121	-	4,4,4	0.37	0	4,4,4	0.57	0
3	DMF	F	249	-	4,4,4	0.34	0	4,4,4	0.43	0
3	DMF	B	249	-	4,4,4	0.31	0	4,4,4	0.46	0
3	DMF	D	249	-	4,4,4	0.33	0	4,4,4	0.49	0
3	DMF	H	142	-	4,4,4	0.38	0	4,4,4	0.51	0
3	DMF	N	21	-	4,4,4	0.32	0	4,4,4	0.44	0
3	DMF	P	107	-	4,4,4	0.29	0	4,4,4	0.43	0
3	DMF	V	135	-	4,4,4	0.41	0	4,4,4	0.46	0
3	DMF	G	137	-	4,4,4	0.36	0	4,4,4	0.46	0
3	DMF	Q	249	-	4,4,4	0.33	0	4,4,4	0.37	0
3	DMF	Y	250	-	4,4,4	0.30	0	4,4,4	0.42	0
3	DMF	G	140	-	4,4,4	0.37	0	4,4,4	0.50	0
3	DMF	O	7	-	4,4,4	0.38	0	4,4,4	0.40	0
3	DMF	T	62	-	4,4,4	0.34	0	4,4,4	0.38	0
3	DMF	Y	251	-	4,4,4	0.41	0	4,4,4	0.47	0
3	DMF	P	133	-	4,4,4	0.35	0	4,4,4	0.49	0
3	DMF	Z	69	-	4,4,4	0.36	0	4,4,4	0.36	0
3	DMF	1	250	-	4,4,4	0.38	0	4,4,4	0.49	0
3	DMF	K	249	-	4,4,4	0.31	0	4,4,4	0.32	0
3	DMF	T	134	-	4,4,4	0.35	0	4,4,4	0.48	0
3	DMF	H	41	-	4,4,4	0.33	0	4,4,4	0.47	0
3	DMF	E	113	-	4,4,4	0.38	0	4,4,4	0.50	0

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	DMF	L	9	-	-	0/2/2/2	-
3	DMF	Z	105	-	-	0/2/2/2	-
3	DMF	M	249	-	-	0/2/2/2	-
3	DMF	S	250	-	-	2/2/2/2	-
3	DMF	X	141	-	-	0/2/2/2	-
3	DMF	2	145	-	-	2/2/2/2	-
3	DMF	K	251	-	-	1/2/2/2	-
3	DMF	A	8	-	-	0/2/2/2	-
3	DMF	V	16	-	-	2/2/2/2	-
3	DMF	Q	250	-	-	0/2/2/2	-
3	DMF	K	250	-	-	2/2/2/2	-
3	DMF	V	136	-	-	0/2/2/2	-
3	DMF	Z	27	-	-	2/2/2/2	-
3	DMF	C	15	-	-	2/2/2/2	-
3	DMF	P	23	-	-	2/2/2/2	-
3	DMF	Q	251	-	-	2/2/2/2	-
3	DMF	L	138	-	-	2/2/2/2	-
3	DMF	I	249	-	-	2/2/2/2	-
3	DMF	U	250	-	-	2/2/2/2	-
3	DMF	N	36	-	-	0/2/2/2	-
3	DMF	L	14	-	-	2/2/2/2	-
3	DMF	U	249	-	-	2/2/2/2	-
3	DMF	A	249	-	-	0/2/2/2	-
3	DMF	E	28	-	-	2/2/2/2	-
3	DMF	Z	50	-	-	2/2/2/2	-
3	DMF	Z	122	-	-	2/2/2/2	-
3	DMF	L	60	-	-	2/2/2/2	-
3	DMF	Y	249	-	-	2/2/2/2	-
3	DMF	1	249	-	-	2/2/2/2	-
3	DMF	W	249	-	-	2/2/2/2	-
3	DMF	E	104	-	-	2/2/2/2	-
3	DMF	J	46	-	-	0/2/2/2	-
3	DMF	V	117	-	-	0/2/2/2	-
3	DMF	G	20	-	-	2/2/2/2	-
3	DMF	2	99	-	-	2/2/2/2	-
3	DMF	S	249	-	-	2/2/2/2	-
3	DMF	V	121	-	-	0/2/2/2	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	DMF	F	249	-	-	2/2/2/2	-
3	DMF	B	249	-	-	1/2/2/2	-
3	DMF	D	249	-	-	0/2/2/2	-
3	DMF	H	142	-	-	2/2/2/2	-
3	DMF	N	21	-	-	2/2/2/2	-
3	DMF	P	107	-	-	2/2/2/2	-
3	DMF	V	135	-	-	2/2/2/2	-
3	DMF	G	137	-	-	2/2/2/2	-
3	DMF	Q	249	-	-	0/2/2/2	-
3	DMF	Y	250	-	-	0/2/2/2	-
3	DMF	G	140	-	-	2/2/2/2	-
3	DMF	O	7	-	-	0/2/2/2	-
3	DMF	T	62	-	-	0/2/2/2	-
3	DMF	Y	251	-	-	2/2/2/2	-
3	DMF	P	133	-	-	2/2/2/2	-
3	DMF	Z	69	-	-	2/2/2/2	-
3	DMF	1	250	-	-	0/2/2/2	-
3	DMF	K	249	-	-	2/2/2/2	-
3	DMF	T	134	-	-	0/2/2/2	-
3	DMF	H	41	-	-	2/2/2/2	-
3	DMF	E	113	-	-	1/2/2/2	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 75 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	2	99	DMF	O-C-N-C2
3	Q	251	DMF	O-C-N-C2
3	2	99	DMF	O-C-N-C1
3	V	16	DMF	O-C-N-C1
3	G	137	DMF	O-C-N-C1

There are no ring outliers.

32 monomers are involved in 55 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	L	9	DMF	1	0
3	Z	105	DMF	2	0
3	2	145	DMF	1	0
3	K	251	DMF	4	0
3	V	16	DMF	1	0
3	V	136	DMF	1	0
3	Q	251	DMF	5	0
3	L	138	DMF	3	0
3	I	249	DMF	1	0
3	U	249	DMF	1	0
3	A	249	DMF	1	0
3	Y	249	DMF	1	0
3	1	249	DMF	2	0
3	W	249	DMF	1	0
3	E	104	DMF	3	0
3	V	117	DMF	1	0
3	G	20	DMF	1	0
3	2	99	DMF	1	0
3	S	249	DMF	1	0
3	V	121	DMF	3	0
3	H	142	DMF	1	0
3	N	21	DMF	1	0
3	P	107	DMF	2	0
3	V	135	DMF	1	0
3	G	137	DMF	1	0
3	G	140	DMF	2	0
3	T	62	DMF	3	0
3	P	133	DMF	1	0
3	Z	69	DMF	5	0
3	K	249	DMF	1	0
3	T	134	DMF	2	0
3	E	113	DMF	1	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, 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	222/240 (92%)	-0.26	2 (0%) 81 78	17, 32, 63, 84	0
1	C	222/240 (92%)	0.72	8 (3%) 46 41	26, 43, 72, 89	0
1	E	223/240 (92%)	-0.13	3 (1%) 75 71	19, 32, 67, 134	0
1	G	222/240 (92%)	-0.37	0 100 100	18, 28, 62, 83	0
1	H	223/240 (92%)	0.16	3 (1%) 75 71	22, 36, 65, 86	0
1	J	222/240 (92%)	0.32	4 (1%) 67 64	24, 38, 71, 89	0
1	L	222/240 (92%)	-0.34	1 (0%) 87 85	18, 30, 64, 83	0
1	N	223/240 (92%)	-0.43	2 (0%) 81 78	15, 30, 64, 118	0
1	P	222/240 (92%)	-0.21	0 100 100	19, 33, 67, 85	0
1	R	222/240 (92%)	-0.13	2 (0%) 81 78	22, 34, 66, 84	0
1	T	223/240 (92%)	-0.23	1 (0%) 88 86	21, 33, 67, 98	0
1	V	226/240 (94%)	-0.39	0 100 100	16, 29, 65, 81	0
1	X	224/240 (93%)	-0.42	2 (0%) 81 78	19, 30, 66, 124	0
1	Z	224/240 (93%)	-0.18	1 (0%) 88 86	21, 34, 68, 107	0
2	1	214/240 (89%)	0.44	11 (5%) 33 29	25, 48, 89, 127	0
2	A	214/240 (89%)	1.30	43 (20%) 3 2	37, 64, 111, 131	0
2	B	214/240 (89%)	2.46	126 (58%) 0 0	40, 87, 134, 168	0
2	D	213/240 (88%)	0.33	13 (6%) 27 23	24, 49, 98, 124	0
2	F	214/240 (89%)	0.36	16 (7%) 20 18	24, 48, 96, 127	0
2	I	214/240 (89%)	1.17	29 (13%) 7 5	34, 53, 98, 125	0
2	K	214/240 (89%)	0.34	5 (2%) 61 57	25, 49, 92, 126	0
2	M	214/240 (89%)	0.20	7 (3%) 49 45	22, 45, 90, 124	0
2	O	214/240 (89%)	0.56	11 (5%) 33 29	26, 54, 95, 129	0
2	Q	214/240 (89%)	0.20	13 (6%) 27 23	20, 42, 90, 126	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
2	S	214/240 (89%)	0.72	16 (7%)	20 18	28, 53, 98, 126	0
2	U	214/240 (89%)	0.67	20 (9%)	14 12	22, 51, 99, 126	0
2	W	214/240 (89%)	0.36	13 (6%)	27 23	22, 46, 94, 125	0
2	Y	214/240 (89%)	0.40	11 (5%)	33 29	23, 46, 90, 127	0
All	All	6115/6720 (90%)	0.26	363 (5%)	28 24	15, 40, 90, 168	0

The worst 5 of 363 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	U	234	LEU	10.9
2	B	180	ALA	6.8
2	B	221	ALA	6.5
2	B	36	ALA	6.3
2	B	31	VAL	6.2

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	DMF	V	135	5/5	0.65	0.29	35,51,75,87	0
3	DMF	Z	69	5/5	0.76	0.21	53,80,102,104	0
3	DMF	Z	27	5/5	0.82	0.21	56,66,86,97	0
3	DMF	H	142	5/5	0.83	0.20	40,62,68,72	0
3	DMF	1	250	5/5	0.83	0.19	43,63,73,87	0
3	DMF	K	251	5/5	0.85	0.15	39,50,64,80	0
3	DMF	L	9	5/5	0.85	0.22	53,54,82,89	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	DMF	U	250	5/5	0.86	0.18	50,54,62,63	0
3	DMF	Y	251	5/5	0.86	0.14	42,45,61,63	0
3	DMF	E	104	5/5	0.86	0.17	33,42,51,57	0
3	DMF	V	117	5/5	0.87	0.16	46,50,66,72	0
3	DMF	S	249	5/5	0.87	0.16	37,57,66,75	0
3	DMF	G	20	5/5	0.87	0.19	27,40,70,93	0
3	DMF	H	41	5/5	0.87	0.16	53,56,63,80	0
3	DMF	L	14	5/5	0.87	0.20	30,38,70,90	0
3	DMF	P	107	5/5	0.88	0.18	39,58,69,70	0
3	DMF	E	113	5/5	0.89	0.19	48,56,75,77	0
3	DMF	Z	50	5/5	0.89	0.26	86,90,126,146	0
3	DMF	T	62	5/5	0.89	0.23	45,61,83,95	0
3	DMF	Y	249	5/5	0.89	0.14	19,24,64,70	0
3	DMF	2	99	5/5	0.89	0.14	33,35,64,80	0
3	DMF	B	249	5/5	0.89	0.12	30,46,52,59	0
3	DMF	V	136	5/5	0.90	0.13	36,44,59,63	0
3	DMF	O	7	5/5	0.90	0.13	38,48,59,62	0
3	DMF	Q	251	5/5	0.90	0.15	26,56,59,84	0
3	DMF	Z	122	5/5	0.90	0.15	26,28,76,84	0
3	DMF	E	28	5/5	0.90	0.16	36,68,72,88	0
3	DMF	A	249	5/5	0.90	0.12	23,35,53,58	0
3	DMF	V	16	5/5	0.90	0.16	36,61,65,73	0
3	DMF	K	250	5/5	0.90	0.13	42,58,73,78	0
3	DMF	N	36	5/5	0.91	0.13	35,43,74,83	0
3	DMF	Q	250	5/5	0.91	0.12	23,37,45,58	0
3	DMF	P	133	5/5	0.91	0.18	62,69,81,113	0
3	DMF	Z	105	5/5	0.91	0.18	22,57,81,82	0
3	DMF	L	60	5/5	0.92	0.12	35,39,50,58	0
3	DMF	C	15	5/5	0.92	0.21	54,69,74,107	0
3	DMF	G	137	5/5	0.92	0.10	27,35,51,57	0
3	DMF	1	249	5/5	0.92	0.15	19,49,53,60	0
3	DMF	2	145	5/5	0.92	0.15	29,42,52,58	0
3	DMF	S	250	5/5	0.93	0.12	26,42,81,85	0
3	DMF	A	8	5/5	0.93	0.15	16,61,76,85	0
3	DMF	L	138	5/5	0.93	0.15	40,47,72,82	0
3	DMF	X	141	5/5	0.93	0.15	40,55,82,85	0
3	DMF	I	249	5/5	0.93	0.14	41,43,50,58	0
3	DMF	G	140	5/5	0.93	0.11	24,33,57,59	0
3	DMF	J	46	5/5	0.94	0.13	29,54,61,63	0
3	DMF	W	249	5/5	0.94	0.10	25,31,39,60	0
3	DMF	N	21	5/5	0.94	0.12	17,53,56,76	0
3	DMF	V	121	5/5	0.94	0.11	26,27,49,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	DMF	T	134	5/5	0.94	0.13	33,56,59,79	0
3	DMF	U	249	5/5	0.94	0.09	11,23,39,54	0
3	DMF	F	249	5/5	0.95	0.08	26,28,37,42	0
3	DMF	P	23	5/5	0.95	0.13	49,62,83,93	0
3	DMF	Y	250	5/5	0.96	0.08	14,36,48,55	0
3	DMF	Q	249	5/5	0.96	0.09	31,39,42,58	0
3	DMF	M	249	5/5	0.96	0.09	12,15,43,51	0
3	DMF	K	249	5/5	0.96	0.09	23,32,46,48	0
3	DMF	D	249	5/5	0.97	0.09	21,22,39,53	0

6.5 Other polymers [i](#)

There are no such residues in this entry.