wwPDB X-ray Structure Validation Summary Report (i)

Apr 29, 2025 – 06:17 AM EDT

PDB ID	:	3H6F / pdb_00003h6f
Title	:	Crystal Structure of Mycobacterium Tuberculosis Proteasome Modified by inhibitor HT1171
Authors	:	Li, D.; Li, H.; Lin, G.
Deposited on	:	2009-04-23
Resolution	:	2.51 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 (i) 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 (i)) were used in the production of this report:

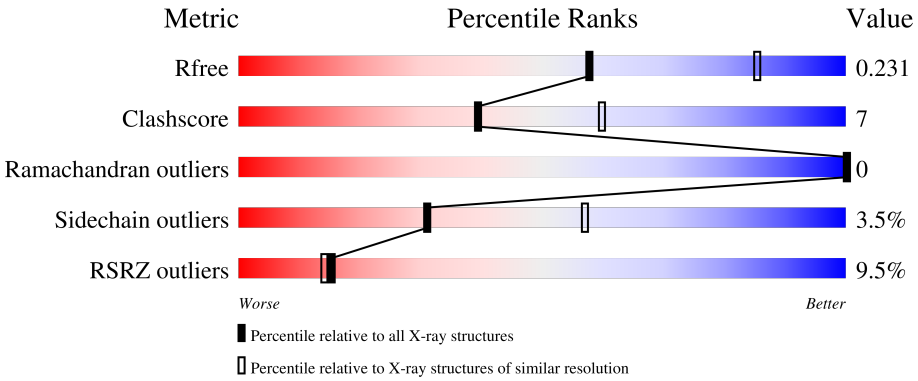
MolProbity	:	4-5-2 with Phenix2.0rc1
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.51 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	5504 (2.50-2.50)
Clashscore	180529	6282 (2.50-2.50)
Ramachandran outliers	177936	6191 (2.50-2.50)
Sidechain outliers	177891	6193 (2.50-2.50)
RSRZ outliers	164620	5504 (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 <=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	13% 74% 11% • 13%
1	A	248	12% 72% 13% • 13%
1	B	248	18% 76% 9% • 14%
1	D	248	14% 72% 13% • 14%
1	F	248	16% 76% 10% • 13%

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Mol	Chain	Length	Quality of chain
1	I	248	13% 71% 13% • 14%
1	K	248	15% 72% 13% • 13%
1	M	248	15% 71% 15% • 13%
1	O	248	12% 74% 12% • 13%
1	Q	248	17% 70% 17% • 12%
1	S	248	12% 71% 15% 13%
1	U	248	14% 71% 13% • 14%
1	W	248	13% 73% 14% • 12%
1	Y	248	22% 71% 12% • 14%
2	2	240	2% 82% 7% 10%
2	C	240	2% 80% 8% • 10%
2	E	240	% 78% 10% • 10%
2	G	240	% 82% 7% • 10%
2	H	240	% 81% 6% • 11%
2	J	240	2% 80% 9% • 10%
2	L	240	2% 82% 7% • 10%
2	N	240	% 79% 8% • 11%
2	P	240	% 81% 8% • 10%
2	R	240	3% 81% 12% 7%
2	T	240	2% 81% 8% 10%
2	V	240	2% 79% 12% • 8%
2	X	240	2% 82% 6% • 10%
2	Z	240	% 80% 10% 10%

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	2	49	-	-	-	X
3	DMF	C	55	-	-	X	-
3	DMF	J	4	-	-	X	-
3	DMF	P	14	-	-	-	X
3	DMF	T	29	-	-	X	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 47697 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 (Alpha subunit) PrcA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	215	Total	C	N	O	S	0	0	0
			1656	1038	303	312	3			
1	B	214	Total	C	N	O	S	0	0	0
			1650	1033	302	312	3			
1	D	214	Total	C	N	O	S	0	0	0
			1648	1032	302	311	3			
1	F	216	Total	C	N	O	S	0	0	0
			1662	1041	304	314	3			
1	I	214	Total	C	N	O	S	0	0	0
			1652	1036	302	311	3			
1	K	215	Total	C	N	O	S	0	0	0
			1656	1038	303	312	3			
1	M	215	Total	C	N	O	S	0	0	0
			1658	1039	303	313	3			
1	O	215	Total	C	N	O	S	0	0	0
			1654	1035	303	313	3			
1	Q	217	Total	C	N	O	S	0	0	0
			1670	1047	305	315	3			
1	S	215	Total	C	N	O	S	0	0	0
			1654	1035	303	313	3			
1	U	214	Total	C	N	O	S	0	0	0
			1650	1033	302	312	3			
1	W	217	Total	C	N	O	S	0	0	0
			1670	1047	305	315	3			
1	Y	213	Total	C	N	O	S	0	0	0
			1644	1030	301	310	3			
1	1	215	Total	C	N	O	S	0	0	0
			1656	1038	303	312	3			

- Molecule 2 is a protein called Proteasome (Beta subunit) PrcB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	215	Total	C	N	O	S	0	0	0
			1593	998	274	317	4			
2	E	216	Total	C	N	O	S	0	0	0
			1601	1004	275	318	4			
2	G	216	Total	C	N	O	S	0	0	0
			1601	1004	275	318	4			
2	H	213	Total	C	N	O	S	0	0	0
			1583	992	272	315	4			
2	J	216	Total	C	N	O	S	0	0	0
			1601	1004	275	318	4			
2	L	216	Total	C	N	O	S	0	0	0
			1601	1004	275	318	4			
2	N	213	Total	C	N	O	S	0	0	0
			1580	989	272	315	4			
2	P	216	Total	C	N	O	S	0	0	0
			1601	1004	275	318	4			
2	R	223	Total	C	N	O	S	0	0	0
			1646	1031	282	329	4			
2	T	216	Total	C	N	O	S	0	0	0
			1601	1004	275	318	4			
2	V	222	Total	C	N	O	S	0	0	0
			1638	1025	281	328	4			
2	X	216	Total	C	N	O	S	0	0	0
			1601	1004	275	318	4			
2	Z	215	Total	C	N	O	S	0	0	0
			1593	998	274	317	4			
2	2	215	Total	C	N	O	S	0	0	0
			1593	998	274	317	4			

There are 98 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	301	OZT	-	insertion	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	-	insertion	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

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Chain	Residue	Modelled	Actual	Comment	Reference
E	539	HIS	-	expression tag	UNP O33245
E	540	HIS	-	expression tag	UNP O33245
G	301	OZT	-	insertion	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
H	301	OZT	-	insertion	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	301	OZT	-	insertion	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	-	insertion	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	-	insertion	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	301	OZT	-	insertion	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	-	insertion	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	-	insertion	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	301	OZT	-	insertion	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	301	OZT	-	insertion	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	-	insertion	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	-	insertion	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

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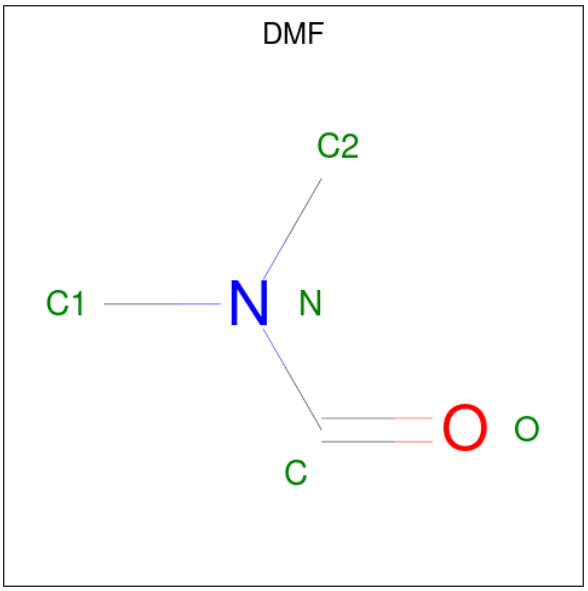
Chain	Residue	Modelled	Actual	Comment	Reference
2	539	HIS	-	expression tag	UNP O33245
2	540	HIS	-	expression tag	UNP O33245

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			5	3	1	1		
3	B	1	Total	C	N	O	0	0
			5	3	1	1		
3	B	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	C	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	C	1	Total	C	N	O	0	0
			5	3	1	1		
3	D	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		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	E	1	Total	C	N	O	0	0
			5	3	1	1		
3	F	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	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	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	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	I	1	Total	C	N	O	0	0
			5	3	1	1		
3	I	1	Total	C	N	O	0	0
			5	3	1	1		
3	J	1	Total	C	N	O	0	0
			5	3	1	1		
3	J	1	Total	C	N	O	0	0
			5	3	1	1		
3	J	1	Total	C	N	O	0	0
			5	3	1	1		
3	K	1	Total	C	N	O	0	0
			5	3	1	1		
3	K	1	Total	C	N	O	0	0
			5	3	1	1		
3	K	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		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	L	1	Total	C	N	O	0	0
			5	3	1	1		
3	M	1	Total	C	N	O	0	0
			5	3	1	1		
3	M	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	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	O	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	P	1	Total	C	N	O	0	0
			5	3	1	1		
3	Q	1	Total	C	N	O	0	0
			5	3	1	1		
3	R	1	Total	C	N	O	0	0
			5	3	1	1		
3	R	1	Total	C	N	O	0	0
			5	3	1	1		
3	S	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	U	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		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	W	1	Total C N O 5 3 1 1	0	0
3	X	1	Total C N O 5 3 1 1	0	0
3	X	1	Total C N O 5 3 1 1	0	0
3	X	1	Total C N O 5 3 1 1	0	0
3	Z	1	Total C N O 5 3 1 1	0	0
3	Z	1	Total C N O 5 3 1 1	0	0
3	Z	1	Total C N O 5 3 1 1	0	0
3	Z	1	Total C N O 5 3 1 1	0	0
3	Z	1	Total C N O 5 3 1 1	0	0
3	1	1	Total C N O 5 3 1 1	0	0
3	1	1	Total C N O 5 3 1 1	0	0
3	2	1	Total C N O 5 3 1 1	0	0
3	2	1	Total C N O 5 3 1 1	0	0
3	2	1	Total C N O 5 3 1 1	0	0
3	2	1	Total C N O 5 3 1 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	34	Total O 34 34	0	0
4	B	40	Total O 40 40	0	0
4	C	95	Total O 95 95	0	0
4	D	49	Total O 49 49	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	E	89	Total O 89 89	0	0
4	F	40	Total O 40 40	0	0
4	G	72	Total O 72 72	0	0
4	H	91	Total O 91 91	0	0
4	I	38	Total O 38 38	0	0
4	J	90	Total O 90 90	0	0
4	K	39	Total O 39 39	0	0
4	L	90	Total O 90 90	0	0
4	M	42	Total O 42 42	0	0
4	N	86	Total O 86 86	0	0
4	O	40	Total O 40 40	0	0
4	P	82	Total O 82 82	0	0
4	Q	34	Total O 34 34	0	0
4	R	97	Total O 97 97	0	0
4	S	34	Total O 34 34	0	0
4	T	78	Total O 78 78	0	0
4	U	38	Total O 38 38	0	0
4	V	104	Total O 104 104	0	0
4	W	27	Total O 27 27	0	0
4	X	84	Total O 84 84	0	0
4	Y	24	Total O 24 24	0	0

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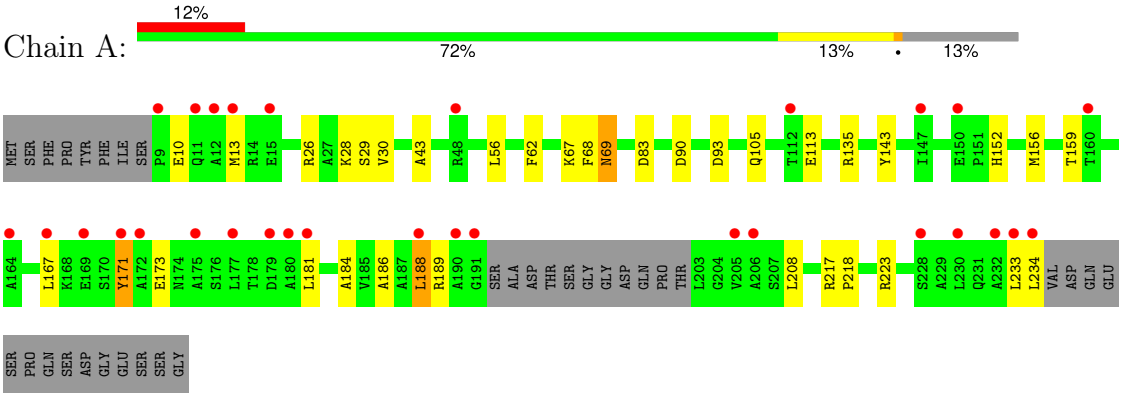
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	Z	85	Total O 85 85	0	0
4	1	34	Total O 34 34	0	0
4	2	93	Total O 93 93	0	0

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.

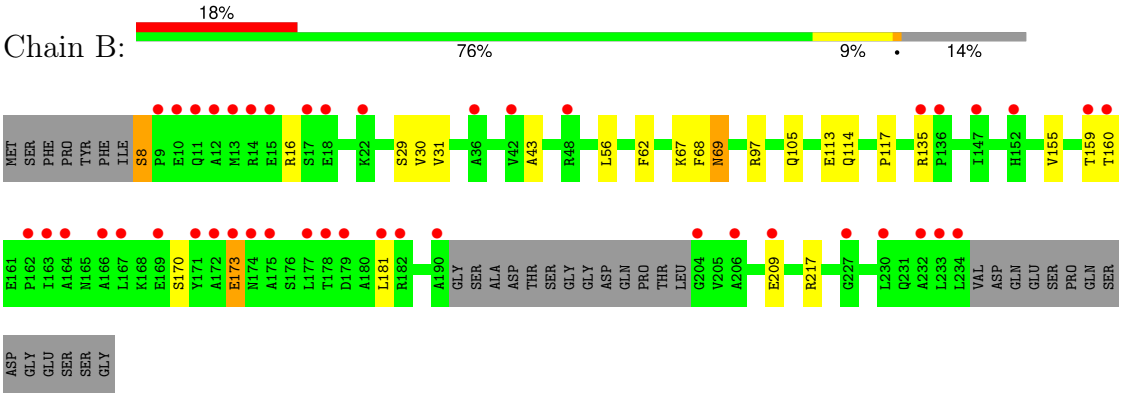
• Molecule 1: Proteasome (Alpha subunit) PrcA

Chain A:



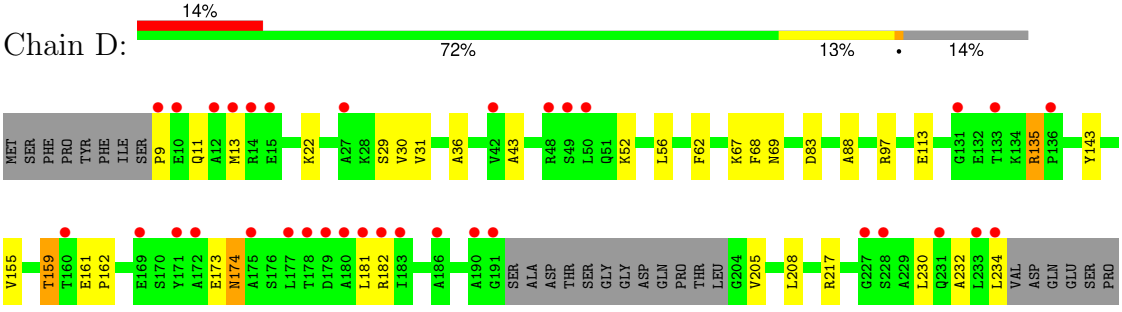
• Molecule 1: Proteasome (Alpha subunit) PrcA

Chain B:



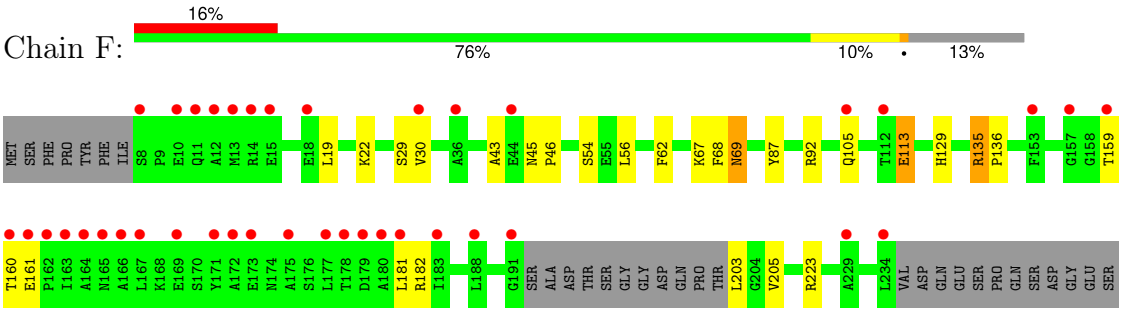
• Molecule 1: Proteasome (Alpha subunit) PrcA

Chain D:



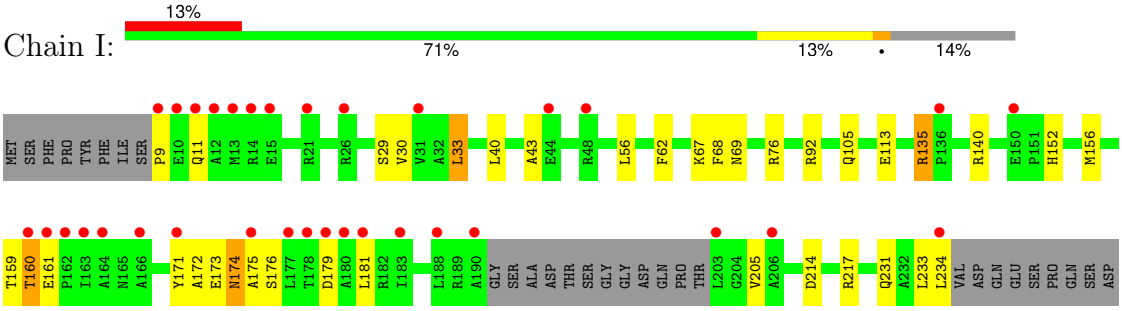
• Molecule 1: Proteasome (Alpha subunit) PrcA

Chain F:



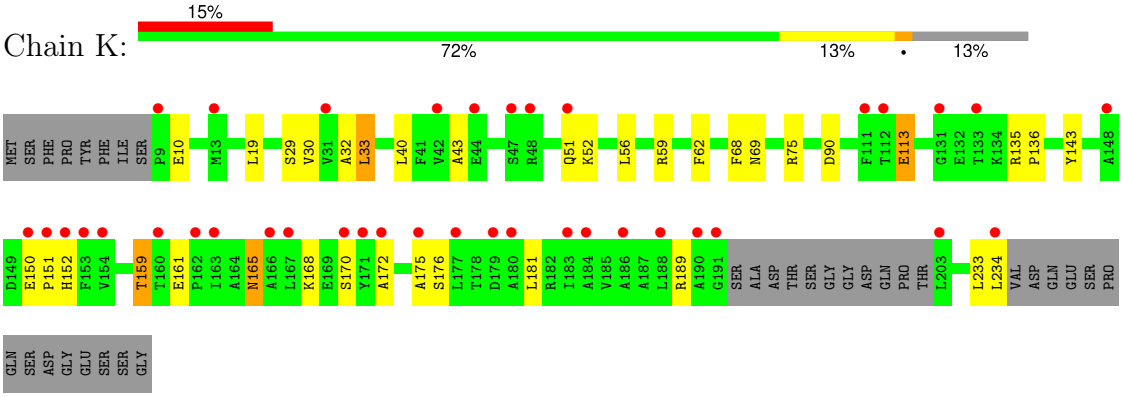
• Molecule 1: Proteasome (Alpha subunit) PrcA

Chain I:



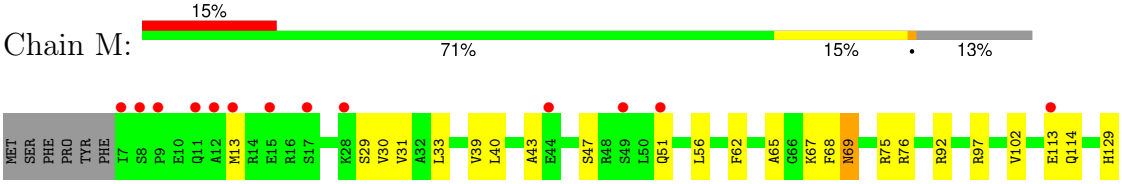
• Molecule 1: Proteasome (Alpha subunit) PrcA

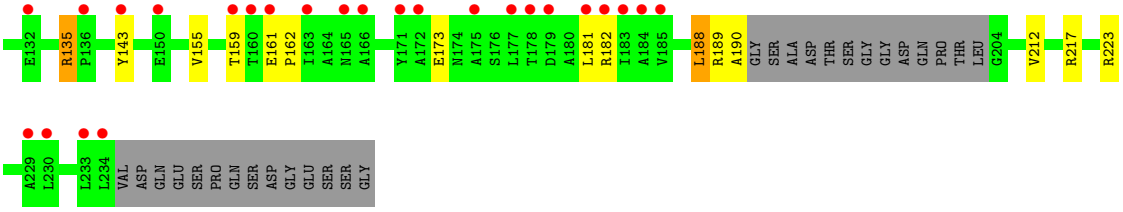
Chain K:



• Molecule 1: Proteasome (Alpha subunit) PrcA

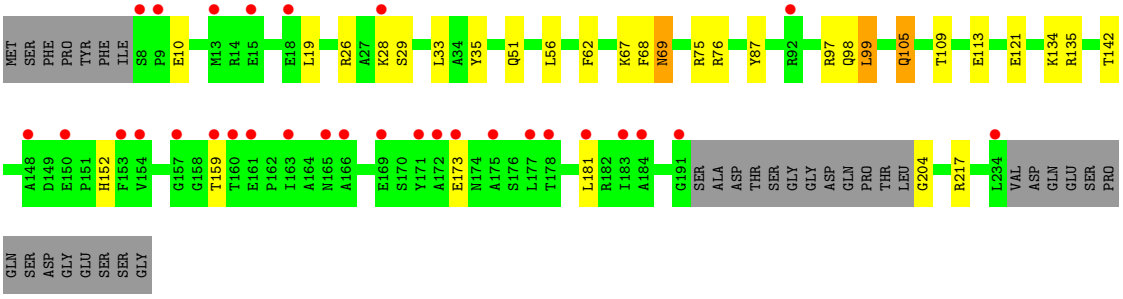
Chain M:





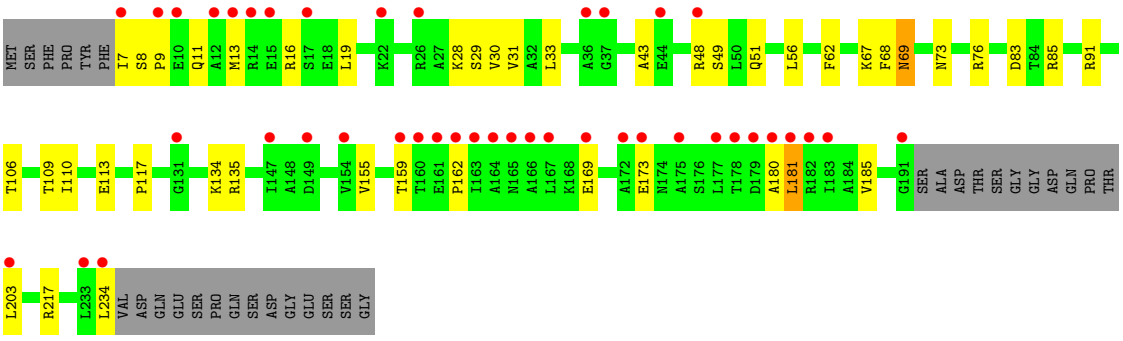
• Molecule 1: Proteasome (Alpha subunit) PrcA

Chain O:



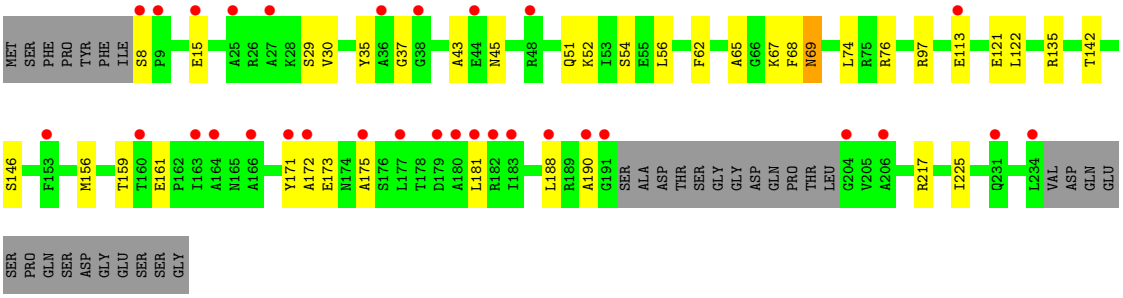
• Molecule 1: Proteasome (Alpha subunit) PrcA

Chain Q:



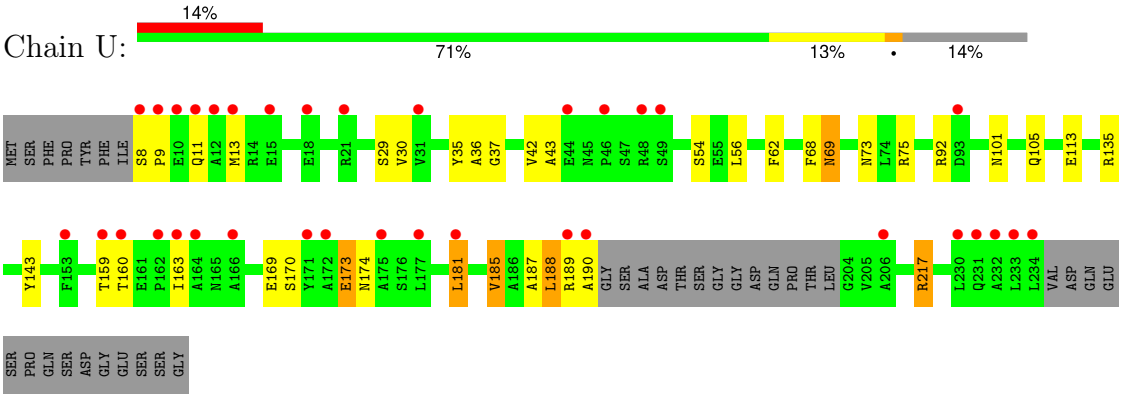
• Molecule 1: Proteasome (Alpha subunit) PrcA

Chain S:



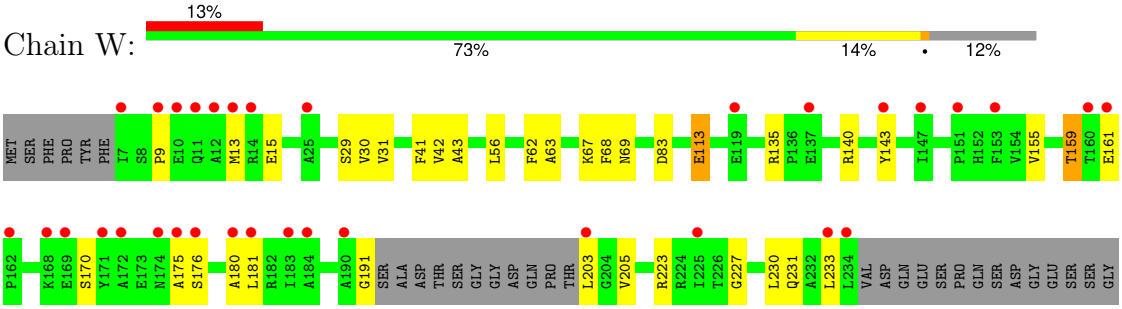
• Molecule 1: Proteasome (Alpha subunit) PrcA

Chain U:



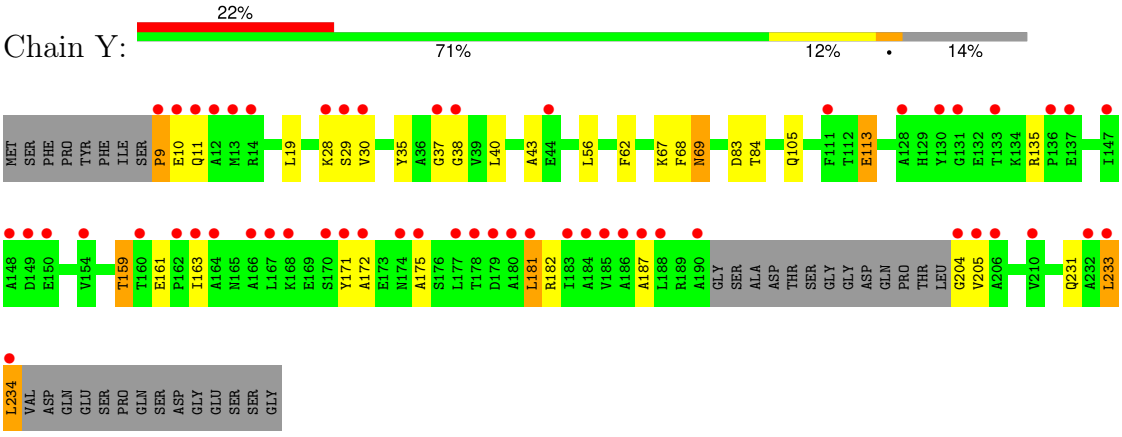
• Molecule 1: Proteasome (Alpha subunit) PrcA

Chain W:



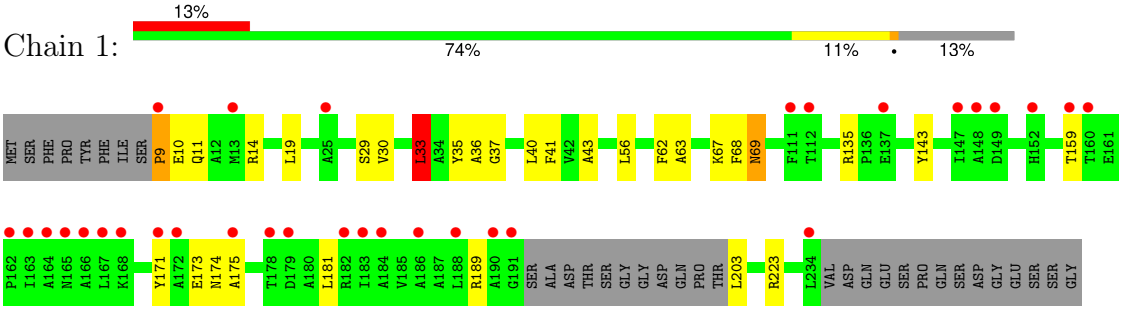
• Molecule 1: Proteasome (Alpha subunit) PrcA

Chain Y:



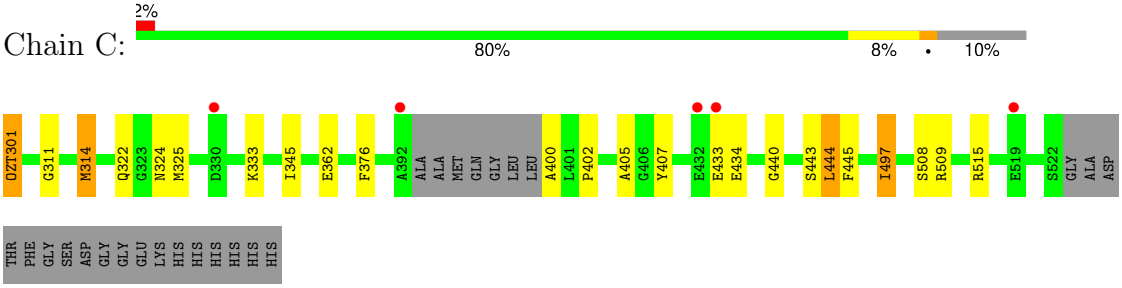
• Molecule 1: Proteasome (Alpha subunit) PrcA

Chain 1:



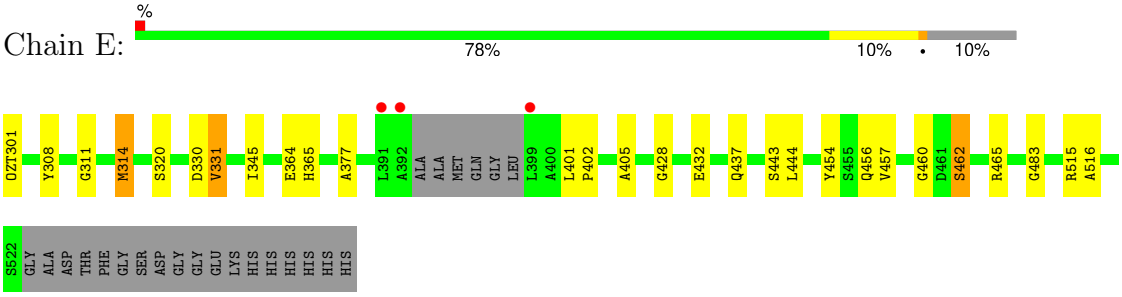
• Molecule 2: Proteasome (Beta subunit) PrcB

Chain C:



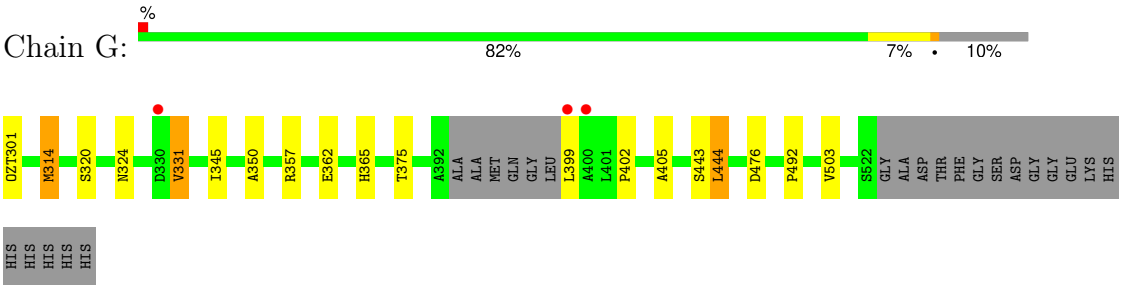
• Molecule 2: Proteasome (Beta subunit) PrcB

Chain E:



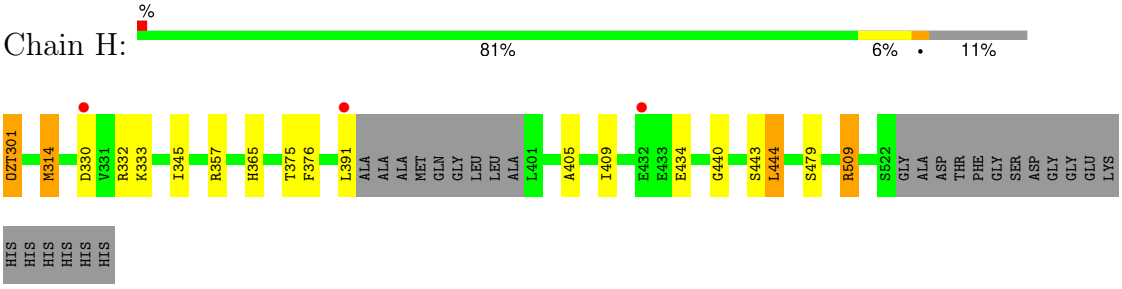
• Molecule 2: Proteasome (Beta subunit) PrcB

Chain G:



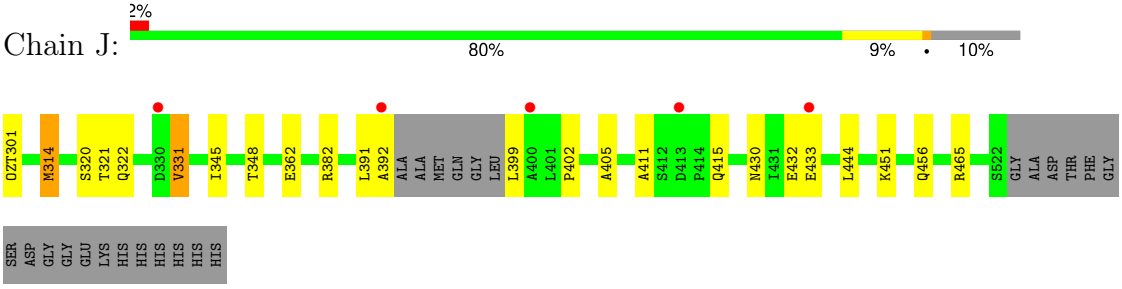
• Molecule 2: Proteasome (Beta subunit) PrcB

Chain H:



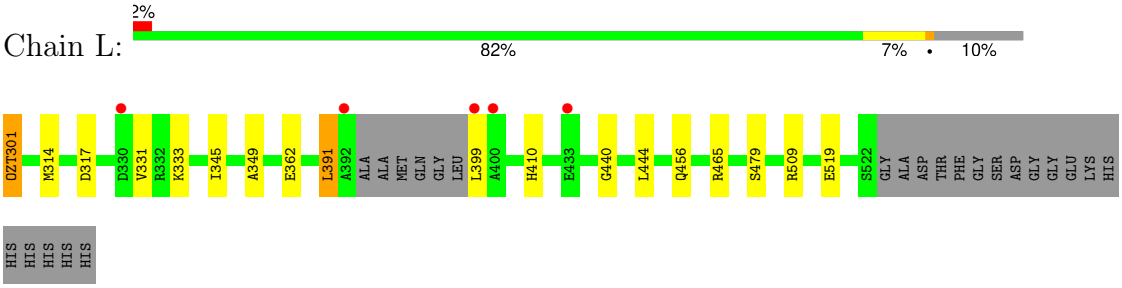
• Molecule 2: Proteasome (Beta subunit) PrcB

Chain J:



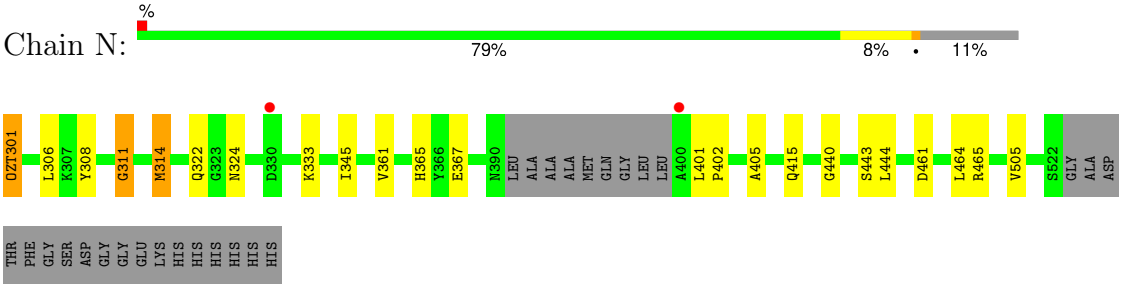
• Molecule 2: Proteasome (Beta subunit) PrcB

Chain L:



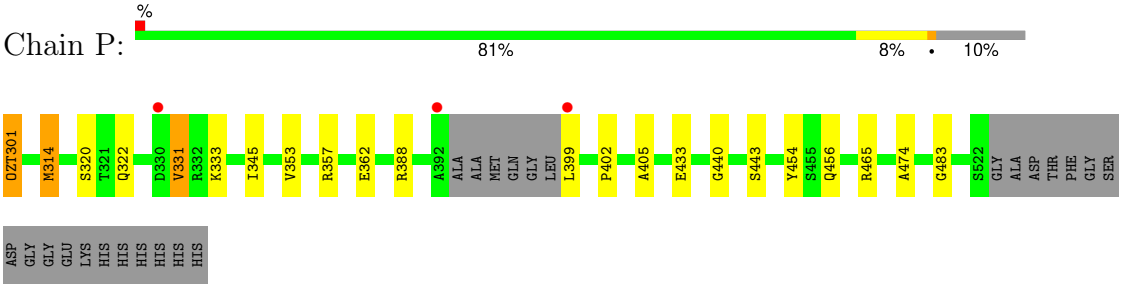
• Molecule 2: Proteasome (Beta subunit) PrcB

Chain N:



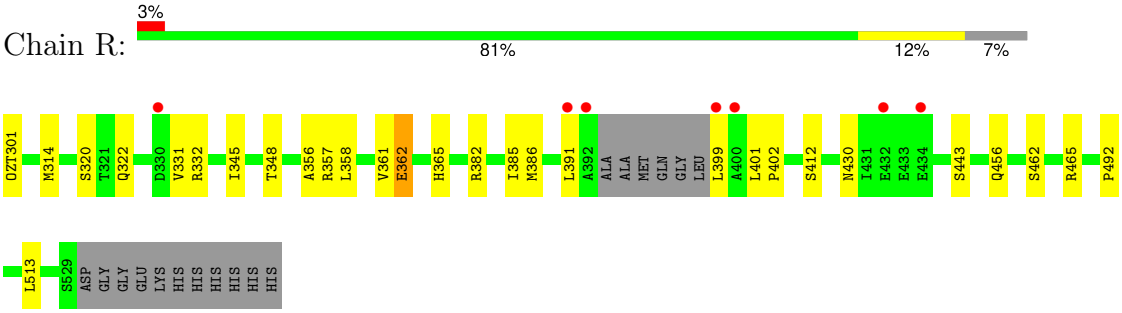
• Molecule 2: Proteasome (Beta subunit) PrcB

Chain P:



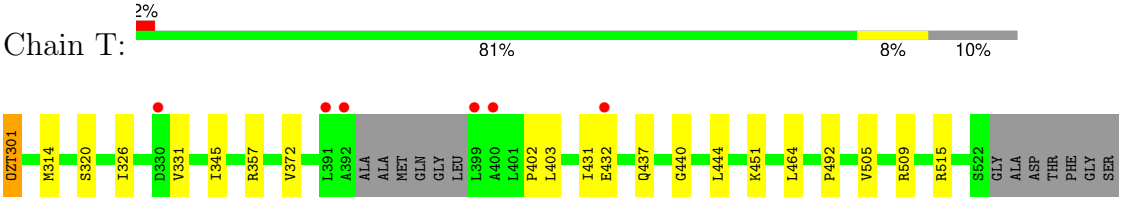
• Molecule 2: Proteasome (Beta subunit) PrcB

Chain R:



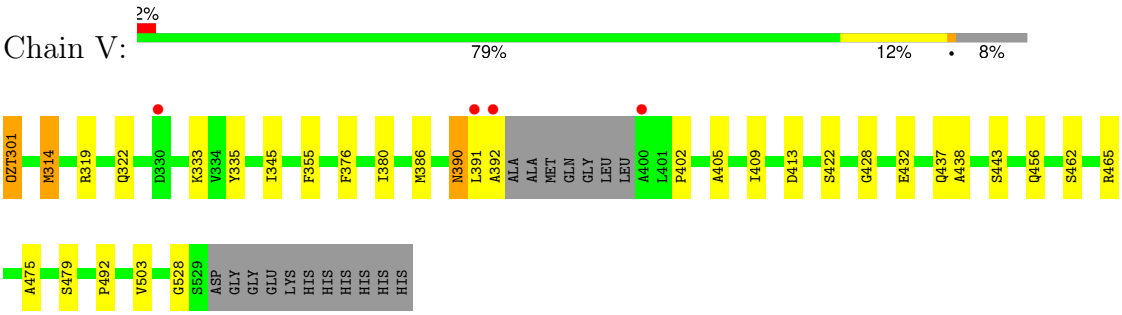
• Molecule 2: Proteasome (Beta subunit) PrcB

Chain T:



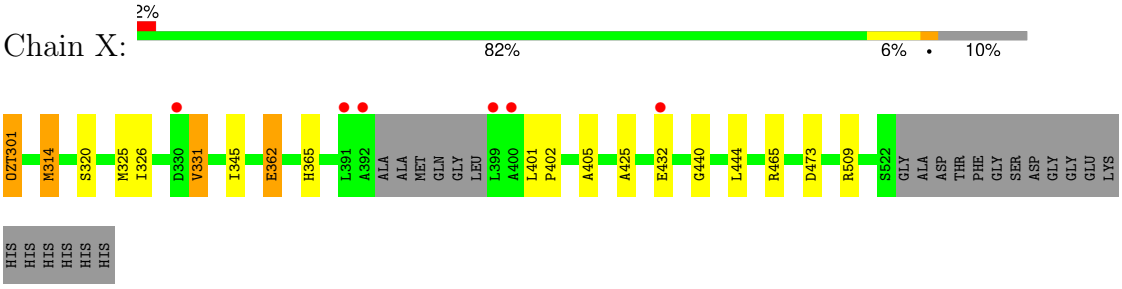
• Molecule 2: Proteasome (Beta subunit) PrcB

Chain V:



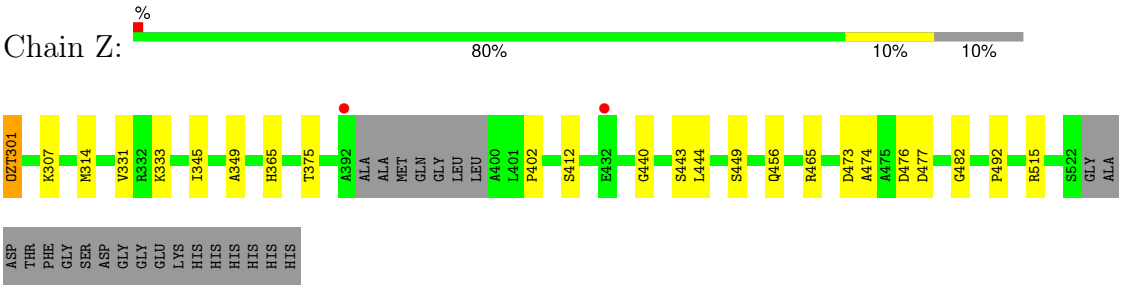
• Molecule 2: Proteasome (Beta subunit) PrcB

Chain X:



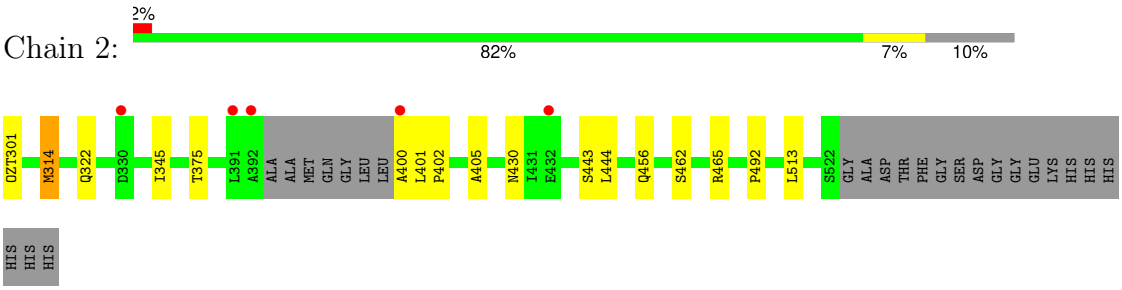
• Molecule 2: Proteasome (Beta subunit) PrcB

Chain Z:



• Molecule 2: Proteasome (Beta subunit) PrcB

Chain 2:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	171.98Å 118.04Å 197.06Å 90.00° 113.62° 90.00°	Depositor
Resolution (Å)	29.83 – 2.51 29.83 – 2.51	Depositor EDS
% Data completeness (in resolution range)	94.2 (29.83-2.51) 94.5 (29.83-2.51)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.84 (at 2.51Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.216 , 0.238 0.211 , 0.231	Depositor DCC
R_{free} test set	11728 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	27.5	Xtriage
Anisotropy	0.239	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 38.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.004 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	47697	wwPDB-VP
Average B, all atoms (Å^2)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.68% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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, 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	1	0.72	0/1681	1.16	8/2270 (0.4%)
1	A	0.76	0/1681	1.11	7/2270 (0.3%)
1	B	0.69	0/1675	1.13	7/2263 (0.3%)
1	D	0.71	0/1673	1.12	5/2259 (0.2%)
1	F	0.72	0/1687	1.09	5/2279 (0.2%)
1	I	0.78	3/1677 (0.2%)	1.15	8/2265 (0.4%)
1	K	0.72	2/1681 (0.1%)	1.10	5/2270 (0.2%)
1	M	0.76	0/1683	1.15	9/2274 (0.4%)
1	O	0.84	0/1679	1.10	5/2268 (0.2%)
1	Q	0.72	0/1695	1.09	4/2290 (0.2%)
1	S	0.67	0/1679	1.10	5/2268 (0.2%)
1	U	0.86	0/1675	1.08	6/2263 (0.3%)
1	W	0.68	0/1695	1.11	6/2290 (0.3%)
1	Y	0.68	0/1669	1.13	8/2254 (0.4%)
2	2	0.87	1/1607 (0.1%)	1.03	2/2178 (0.1%)
2	C	0.91	2/1607 (0.1%)	1.06	5/2178 (0.2%)
2	E	0.97	3/1615 (0.2%)	1.09	6/2189 (0.3%)
2	G	0.80	1/1615 (0.1%)	1.05	4/2189 (0.2%)
2	H	0.83	1/1597 (0.1%)	1.06	2/2164 (0.1%)
2	J	0.90	1/1615 (0.1%)	1.03	2/2189 (0.1%)
2	L	0.90	1/1615 (0.1%)	1.07	0/2189
2	N	0.88	1/1594 (0.1%)	1.05	3/2160 (0.1%)
2	P	0.88	3/1615 (0.2%)	1.05	4/2189 (0.2%)
2	R	0.94	1/1661 (0.1%)	1.07	4/2251 (0.2%)
2	T	0.96	3/1615 (0.2%)	1.08	2/2189 (0.1%)
2	V	0.92	2/1653 (0.1%)	1.07	7/2240 (0.3%)
2	X	0.87	2/1615 (0.1%)	1.04	1/2189 (0.0%)
2	Z	0.93	3/1607 (0.2%)	1.07	4/2178 (0.2%)
All	All	0.82	30/46161 (0.1%)	1.09	134/62455 (0.2%)

The worst 5 of 30 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	314	MET	SD-CE	-10.12	1.54	1.79
2	T	314	MET	SD-CE	-9.03	1.56	1.79
2	2	314	MET	SD-CE	-8.96	1.57	1.79
2	R	314	MET	SD-CE	-8.91	1.57	1.79
2	V	314	MET	SD-CE	-8.67	1.57	1.79

The worst 5 of 134 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1	10	GLU	N-CA-C	-12.23	98.53	114.31
1	Y	10	GLU	N-CA-C	-9.40	101.23	112.89
1	I	160	THR	N-CA-C	8.77	120.92	111.36
2	V	528	GLY	N-CA-C	8.35	124.34	112.82
1	B	173	GLU	N-CA-C	8.15	120.97	111.02

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	1656	0	1658	25	0
1	A	1656	0	1658	24	0
1	B	1650	0	1648	21	0
1	D	1648	0	1647	39	0
1	F	1662	0	1662	23	0
1	I	1652	0	1655	20	0
1	K	1656	0	1658	32	0
1	M	1658	0	1659	41	0
1	O	1654	0	1651	32	0
1	Q	1670	0	1673	42	0
1	S	1654	0	1651	31	0
1	U	1650	0	1648	26	0
1	W	1670	0	1673	25	0
1	Y	1644	0	1644	38	0
2	2	1593	0	1577	12	0
2	C	1593	0	1577	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	1601	0	1588	16	0
2	G	1601	0	1588	10	0
2	H	1583	0	1567	16	0
2	J	1601	0	1588	18	0
2	L	1601	0	1588	9	0
2	N	1580	0	1561	14	0
2	P	1601	0	1588	12	0
2	R	1646	0	1624	21	0
2	T	1601	0	1588	10	0
2	V	1638	0	1613	23	0
2	X	1601	0	1588	16	0
2	Z	1593	0	1577	14	0
3	1	10	0	14	0	0
3	2	20	0	28	0	0
3	A	5	0	7	0	0
3	B	10	0	14	0	0
3	C	20	0	28	6	0
3	D	5	0	7	0	0
3	E	15	0	21	3	0
3	F	5	0	7	0	0
3	G	25	0	35	2	0
3	H	20	0	28	0	0
3	I	10	0	14	0	0
3	J	15	0	21	5	0
3	K	15	0	21	1	0
3	L	15	0	21	2	0
3	M	10	0	14	2	0
3	N	20	0	28	1	0
3	O	5	0	7	0	0
3	P	20	0	28	1	0
3	Q	5	0	7	0	0
3	R	10	0	14	2	0
3	S	5	0	7	0	0
3	T	10	0	14	4	0
3	U	5	0	7	0	0
3	V	10	0	14	1	0
3	W	5	0	7	0	0
3	X	15	0	21	1	0
3	Z	25	0	35	2	0
4	1	34	0	0	9	0
4	2	93	0	0	4	0
4	A	34	0	0	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	40	0	0	13	0
4	C	95	0	0	8	0
4	D	49	0	0	11	0
4	E	89	0	0	5	0
4	F	40	0	0	15	0
4	G	72	0	0	4	0
4	H	91	0	0	11	0
4	I	38	0	0	10	0
4	J	90	0	0	13	0
4	K	39	0	0	18	0
4	L	90	0	0	4	0
4	M	42	0	0	22	0
4	N	86	0	0	4	0
4	O	40	0	0	18	0
4	P	82	0	0	4	0
4	Q	34	0	0	14	0
4	R	97	0	0	5	0
4	S	34	0	0	18	0
4	T	78	0	0	9	0
4	U	38	0	0	7	0
4	V	104	0	0	4	0
4	W	27	0	0	11	0
4	X	84	0	0	10	0
4	Y	24	0	0	14	0
4	Z	85	0	0	7	0
All	All	47697	0	45866	610	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 7.

The worst 5 of 610 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:173:GLU:C	1:D:174:ASN:HD22	1.40	1.29
2:J:432:GLU:HG2	4:J:1761:HOH:O	1.37	1.21
1:I:140:ARG:HD2	4:I:1512:HOH:O	1.41	1.19
2:P:399:LEU:HD12	4:P:1556:HOH:O	1.36	1.19
2:E:432:GLU:HG2	4:E:1322:HOH:O	1.42	1.18

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%)	205 (97%)	6 (3%)	0	100	100
1	A	211/248 (85%)	204 (97%)	7 (3%)	0	100	100
1	B	210/248 (85%)	205 (98%)	5 (2%)	0	100	100
1	D	210/248 (85%)	205 (98%)	5 (2%)	0	100	100
1	F	212/248 (86%)	207 (98%)	5 (2%)	0	100	100
1	I	210/248 (85%)	204 (97%)	6 (3%)	0	100	100
1	K	211/248 (85%)	206 (98%)	5 (2%)	0	100	100
1	M	211/248 (85%)	205 (97%)	6 (3%)	0	100	100
1	O	211/248 (85%)	207 (98%)	4 (2%)	0	100	100
1	Q	213/248 (86%)	207 (97%)	6 (3%)	0	100	100
1	S	211/248 (85%)	207 (98%)	4 (2%)	0	100	100
1	U	210/248 (85%)	205 (98%)	5 (2%)	0	100	100
1	W	213/248 (86%)	207 (97%)	6 (3%)	0	100	100
1	Y	209/248 (84%)	202 (97%)	7 (3%)	0	100	100
2	2	211/240 (88%)	209 (99%)	2 (1%)	0	100	100
2	C	211/240 (88%)	209 (99%)	2 (1%)	0	100	100
2	E	212/240 (88%)	210 (99%)	2 (1%)	0	100	100
2	G	212/240 (88%)	208 (98%)	4 (2%)	0	100	100
2	H	209/240 (87%)	206 (99%)	3 (1%)	0	100	100
2	J	212/240 (88%)	209 (99%)	3 (1%)	0	100	100
2	L	212/240 (88%)	210 (99%)	2 (1%)	0	100	100
2	N	209/240 (87%)	208 (100%)	1 (0%)	0	100	100
2	P	212/240 (88%)	209 (99%)	3 (1%)	0	100	100
2	R	219/240 (91%)	217 (99%)	2 (1%)	0	100	100
2	T	212/240 (88%)	210 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	V	218/240 (91%)	216 (99%)	2 (1%)	0	100	100
2	X	212/240 (88%)	208 (98%)	4 (2%)	0	100	100
2	Z	211/240 (88%)	209 (99%)	2 (1%)	0	100	100
All	All	5925/6832 (87%)	5814 (98%)	111 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	1	164/192 (85%)	159 (97%)	5 (3%)	36	63
1	A	164/192 (85%)	156 (95%)	8 (5%)	21	42
1	B	164/192 (85%)	160 (98%)	4 (2%)	44	70
1	D	163/192 (85%)	158 (97%)	5 (3%)	35	62
1	F	165/192 (86%)	160 (97%)	5 (3%)	36	63
1	I	164/192 (85%)	156 (95%)	8 (5%)	21	42
1	K	164/192 (85%)	155 (94%)	9 (6%)	18	37
1	M	165/192 (86%)	159 (96%)	6 (4%)	30	56
1	O	164/192 (85%)	156 (95%)	8 (5%)	21	42
1	Q	166/192 (86%)	158 (95%)	8 (5%)	21	43
1	S	164/192 (85%)	160 (98%)	4 (2%)	44	70
1	U	164/192 (85%)	153 (93%)	11 (7%)	13	28
1	W	166/192 (86%)	159 (96%)	7 (4%)	25	49
1	Y	163/192 (85%)	155 (95%)	8 (5%)	21	42
2	2	160/177 (90%)	156 (98%)	4 (2%)	42	69
2	C	160/177 (90%)	153 (96%)	7 (4%)	24	47
2	E	161/177 (91%)	156 (97%)	5 (3%)	35	62
2	G	161/177 (91%)	156 (97%)	5 (3%)	35	62

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	H	160/177 (90%)	155 (97%)	5 (3%)	35	62
2	J	161/177 (91%)	158 (98%)	3 (2%)	52	77
2	L	161/177 (91%)	156 (97%)	5 (3%)	35	62
2	N	159/177 (90%)	154 (97%)	5 (3%)	35	62
2	P	161/177 (91%)	157 (98%)	4 (2%)	42	69
2	R	165/177 (93%)	160 (97%)	5 (3%)	36	63
2	T	161/177 (91%)	157 (98%)	4 (2%)	42	69
2	V	164/177 (93%)	159 (97%)	5 (3%)	36	63
2	X	161/177 (91%)	159 (99%)	2 (1%)	67	86
2	Z	160/177 (90%)	157 (98%)	3 (2%)	52	77
All	All	4555/5166 (88%)	4397 (96%)	158 (4%)	31	57

5 of 158 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	U	113	GLU
1	Y	181	LEU
1	U	173	GLU
1	W	135	ARG
1	1	69	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 98 such sidechains are listed below:

Mol	Chain	Res	Type
1	Q	114	GLN
1	U	114	GLN
2	R	365	HIS
1	S	114	GLN
2	V	437	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

14 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	$\#\|Z\| > 2$
2	OZT	C	301	2	6,9,10	4.56	3 (50%)	9,12,14	5.97	7 (77%)
2	OZT	N	301	2	6,9,10	4.23	3 (50%)	9,12,14	6.01	7 (77%)
2	OZT	P	301	2	6,9,10	4.09	3 (50%)	9,12,14	6.06	7 (77%)
2	OZT	L	301	2	6,9,10	4.52	3 (50%)	9,12,14	6.08	7 (77%)
2	OZT	V	301	2	6,9,10	4.32	3 (50%)	9,12,14	6.24	7 (77%)
2	OZT	Z	301	2	6,9,10	4.25	3 (50%)	9,12,14	6.04	6 (66%)
2	OZT	J	301	2	6,9,10	4.40	3 (50%)	9,12,14	6.09	7 (77%)
2	OZT	H	301	2	6,9,10	4.25	3 (50%)	9,12,14	6.11	6 (66%)
2	OZT	R	301	2	6,9,10	4.58	3 (50%)	9,12,14	5.79	7 (77%)
2	OZT	X	301	2	6,9,10	4.13	3 (50%)	9,12,14	5.93	6 (66%)
2	OZT	G	301	2	6,9,10	4.17	2 (33%)	9,12,14	5.87	7 (77%)
2	OZT	T	301	2	6,9,10	4.30	3 (50%)	9,12,14	6.12	7 (77%)
2	OZT	E	301	2	6,9,10	4.57	3 (50%)	9,12,14	5.72	7 (77%)
2	OZT	2	301	2	6,9,10	4.05	3 (50%)	9,12,14	6.01	7 (77%)

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
2	OZT	C	301	2	-	1/1/14/16	0/1/1/1
2	OZT	N	301	2	-	1/1/14/16	0/1/1/1
2	OZT	P	301	2	-	1/1/14/16	0/1/1/1
2	OZT	L	301	2	-	1/1/14/16	0/1/1/1
2	OZT	V	301	2	-	1/1/14/16	0/1/1/1
2	OZT	Z	301	2	-	1/1/14/16	0/1/1/1
2	OZT	J	301	2	-	1/1/14/16	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	OZT	H	301	2	-	1/1/14/16	0/1/1/1
2	OZT	R	301	2	-	1/1/14/16	0/1/1/1
2	OZT	X	301	2	-	1/1/14/16	0/1/1/1
2	OZT	G	301	2	-	1/1/14/16	0/1/1/1
2	OZT	T	301	2	-	1/1/14/16	0/1/1/1
2	OZT	E	301	2	-	1/1/14/16	0/1/1/1
2	OZT	2	301	2	-	1/1/14/16	0/1/1/1

The worst 5 of 41 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	301	OZT	O1-C5	10.10	1.49	1.36
2	C	301	OZT	O1-C5	9.91	1.49	1.36
2	R	301	OZT	O1-C5	9.89	1.49	1.36
2	L	301	OZT	O1-C5	9.77	1.49	1.36
2	J	301	OZT	O1-C5	9.52	1.49	1.36

The worst 5 of 95 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	T	301	OZT	O1-C5-N	10.01	118.03	109.87
2	J	301	OZT	O1-C5-N	9.80	117.86	109.87
2	2	301	OZT	O1-C5-N	9.69	117.77	109.87
2	L	301	OZT	O1-C5-N	9.69	117.76	109.87
2	N	301	OZT	O1-C5-N	9.68	117.75	109.87

There are no chirality outliers.

5 of 14 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	2	301	OZT	O-C-CA-C2
2	C	301	OZT	O-C-CA-C2
2	E	301	OZT	O-C-CA-C2
2	G	301	OZT	O-C-CA-C2
2	H	301	OZT	O-C-CA-C2

There are no ring outliers.

9 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	301	OZT	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	N	301	OZT	2	0
2	P	301	OZT	2	0
2	L	301	OZT	1	0
2	V	301	OZT	2	0
2	Z	301	OZT	2	0
2	H	301	OZT	2	0
2	X	301	OZT	1	0
2	T	301	OZT	1	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

67 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	E	20	-	4,4,4	0.58	0	4,4,4	0.35	0
3	DMF	P	56	-	4,4,4	0.50	0	4,4,4	0.32	0
3	DMF	G	60	-	4,4,4	0.56	0	4,4,4	0.38	0
3	DMF	K	250	-	4,4,4	0.61	0	4,4,4	0.40	0
3	DMF	H	32	-	4,4,4	0.69	0	4,4,4	0.37	0
3	DMF	1	250	-	4,4,4	0.60	0	4,4,4	0.30	0
3	DMF	C	47	-	4,4,4	0.55	0	4,4,4	0.39	0
3	DMF	X	61	-	4,4,4	0.43	0	4,4,4	0.39	0
3	DMF	R	59	-	4,4,4	0.64	0	4,4,4	0.37	0
3	DMF	J	45	-	4,4,4	0.60	0	4,4,4	0.38	0
3	DMF	N	22	-	4,4,4	0.58	0	4,4,4	0.33	0
3	DMF	Z	41	-	4,4,4	0.54	0	4,4,4	0.34	0
3	DMF	Z	43	-	4,4,4	0.63	0	4,4,4	0.30	0
3	DMF	2	49	-	4,4,4	0.54	0	4,4,4	0.37	0
3	DMF	I	249	-	4,4,4	0.67	0	4,4,4	0.30	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	DMF	2	52	-	4,4,4	0.55	0	4,4,4	0.31	0
3	DMF	Z	54	-	4,4,4	0.55	0	4,4,4	0.34	0
3	DMF	K	249	-	4,4,4	0.55	0	4,4,4	0.31	0
3	DMF	O	249	-	4,4,4	0.45	0	4,4,4	0.36	0
3	DMF	L	36	-	4,4,4	0.46	0	4,4,4	0.39	0
3	DMF	V	27	-	4,4,4	0.24	0	4,4,4	0.49	0
3	DMF	Z	30	-	4,4,4	0.42	0	4,4,4	0.35	0
3	DMF	1	249	-	4,4,4	0.59	0	4,4,4	0.32	0
3	DMF	X	40	-	4,4,4	0.64	0	4,4,4	0.33	0
3	DMF	H	62	-	4,4,4	0.71	0	4,4,4	0.36	0
3	DMF	F	249	-	4,4,4	0.56	0	4,4,4	0.32	0
3	DMF	I	250	-	4,4,4	0.56	0	4,4,4	0.30	0
3	DMF	K	251	-	4,4,4	0.48	0	4,4,4	0.32	0
3	DMF	P	51	-	4,4,4	0.70	0	4,4,4	0.33	0
3	DMF	R	34	-	4,4,4	0.17	0	4,4,4	0.48	0
3	DMF	S	249	-	4,4,4	0.54	0	4,4,4	0.29	0
3	DMF	X	16	-	4,4,4	0.53	0	4,4,4	0.35	0
3	DMF	Z	18	-	4,4,4	0.45	0	4,4,4	0.37	0
3	DMF	A	249	-	4,4,4	0.50	0	4,4,4	0.30	0
3	DMF	U	249	-	4,4,4	0.46	0	4,4,4	0.31	0
3	DMF	E	66	-	4,4,4	0.68	0	4,4,4	0.33	0
3	DMF	2	42	-	4,4,4	0.37	0	4,4,4	0.34	0
3	DMF	L	53	-	4,4,4	0.50	0	4,4,4	0.39	0
3	DMF	B	250	-	4,4,4	0.59	0	4,4,4	0.32	0
3	DMF	C	10	-	4,4,4	0.49	0	4,4,4	0.42	0
3	DMF	N	2	-	4,4,4	0.56	0	4,4,4	0.29	0
3	DMF	P	65	-	4,4,4	0.64	0	4,4,4	0.34	0
3	DMF	N	15	-	4,4,4	0.48	0	4,4,4	0.30	0
3	DMF	W	249	-	4,4,4	0.52	0	4,4,4	0.33	0
3	DMF	C	38	-	4,4,4	0.26	0	4,4,4	0.35	0
3	DMF	L	3	-	4,4,4	0.31	0	4,4,4	0.33	0
3	DMF	G	24	-	4,4,4	0.54	0	4,4,4	0.30	0
3	DMF	H	33	-	4,4,4	0.63	0	4,4,4	0.39	0
3	DMF	J	4	-	4,4,4	0.54	0	4,4,4	0.36	0
3	DMF	M	250	-	4,4,4	0.75	0	4,4,4	0.38	0
3	DMF	C	55	-	4,4,4	0.30	0	4,4,4	0.60	0
3	DMF	T	67	-	4,4,4	0.56	0	4,4,4	1.28	0
3	DMF	E	28	-	4,4,4	0.61	0	4,4,4	0.31	0
3	DMF	M	249	-	4,4,4	0.52	0	4,4,4	0.35	0
3	DMF	G	64	-	4,4,4	0.57	0	4,4,4	0.42	0
3	DMF	V	39	-	4,4,4	0.62	0	4,4,4	0.34	0
3	DMF	N	58	-	4,4,4	0.52	0	4,4,4	0.38	0
3	DMF	2	63	-	4,4,4	0.61	0	4,4,4	0.39	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	DMF	G	1	-	4,4,4	0.41	0	4,4,4	0.44	0
3	DMF	G	12	-	4,4,4	0.54	0	4,4,4	0.30	0
3	DMF	P	14	-	4,4,4	0.52	0	4,4,4	0.31	0
3	DMF	B	249	-	4,4,4	0.64	0	4,4,4	0.30	0
3	DMF	Q	249	-	4,4,4	0.65	0	4,4,4	0.31	0
3	DMF	D	249	-	4,4,4	0.51	0	4,4,4	0.38	0
3	DMF	J	50	-	4,4,4	0.49	0	4,4,4	0.33	0
3	DMF	T	29	-	4,4,4	0.55	0	4,4,4	0.33	0
3	DMF	H	26	-	4,4,4	0.60	0	4,4,4	0.32	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	E	20	-	-	0/2/2/2	-
3	DMF	P	56	-	-	0/2/2/2	-
3	DMF	G	60	-	-	0/2/2/2	-
3	DMF	K	250	-	-	0/2/2/2	-
3	DMF	H	32	-	-	0/2/2/2	-
3	DMF	1	250	-	-	0/2/2/2	-
3	DMF	C	47	-	-	0/2/2/2	-
3	DMF	X	61	-	-	0/2/2/2	-
3	DMF	R	59	-	-	0/2/2/2	-
3	DMF	J	45	-	-	0/2/2/2	-
3	DMF	N	22	-	-	0/2/2/2	-
3	DMF	Z	41	-	-	0/2/2/2	-
3	DMF	Z	43	-	-	0/2/2/2	-
3	DMF	2	49	-	-	0/2/2/2	-
3	DMF	I	249	-	-	0/2/2/2	-
3	DMF	2	52	-	-	0/2/2/2	-
3	DMF	Z	54	-	-	0/2/2/2	-
3	DMF	K	249	-	-	0/2/2/2	-
3	DMF	O	249	-	-	0/2/2/2	-
3	DMF	L	36	-	-	0/2/2/2	-
3	DMF	V	27	-	-	2/2/2/2	-
3	DMF	Z	30	-	-	0/2/2/2	-
3	DMF	1	249	-	-	0/2/2/2	-
3	DMF	X	40	-	-	0/2/2/2	-
3	DMF	H	62	-	-	0/2/2/2	-
3	DMF	F	249	-	-	0/2/2/2	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	DMF	I	250	-	-	0/2/2/2	-
3	DMF	K	251	-	-	0/2/2/2	-
3	DMF	P	51	-	-	0/2/2/2	-
3	DMF	R	34	-	-	2/2/2/2	-
3	DMF	S	249	-	-	0/2/2/2	-
3	DMF	X	16	-	-	0/2/2/2	-
3	DMF	Z	18	-	-	0/2/2/2	-
3	DMF	A	249	-	-	0/2/2/2	-
3	DMF	U	249	-	-	0/2/2/2	-
3	DMF	E	66	-	-	0/2/2/2	-
3	DMF	2	42	-	-	0/2/2/2	-
3	DMF	L	53	-	-	0/2/2/2	-
3	DMF	B	250	-	-	0/2/2/2	-
3	DMF	C	10	-	-	0/2/2/2	-
3	DMF	N	2	-	-	0/2/2/2	-
3	DMF	P	65	-	-	0/2/2/2	-
3	DMF	N	15	-	-	0/2/2/2	-
3	DMF	W	249	-	-	0/2/2/2	-
3	DMF	C	38	-	-	2/2/2/2	-
3	DMF	L	3	-	-	0/2/2/2	-
3	DMF	G	24	-	-	0/2/2/2	-
3	DMF	H	33	-	-	0/2/2/2	-
3	DMF	J	4	-	-	0/2/2/2	-
3	DMF	M	250	-	-	0/2/2/2	-
3	DMF	C	55	-	-	2/2/2/2	-
3	DMF	T	67	-	-	2/2/2/2	-
3	DMF	E	28	-	-	0/2/2/2	-
3	DMF	M	249	-	-	0/2/2/2	-
3	DMF	G	64	-	-	0/2/2/2	-
3	DMF	V	39	-	-	0/2/2/2	-
3	DMF	N	58	-	-	0/2/2/2	-
3	DMF	2	63	-	-	0/2/2/2	-
3	DMF	G	1	-	-	0/2/2/2	-
3	DMF	G	12	-	-	0/2/2/2	-
3	DMF	P	14	-	-	0/2/2/2	-
3	DMF	B	249	-	-	0/2/2/2	-
3	DMF	Q	249	-	-	0/2/2/2	-
3	DMF	D	249	-	-	0/2/2/2	-
3	DMF	J	50	-	-	0/2/2/2	-
3	DMF	T	29	-	-	0/2/2/2	-
3	DMF	H	26	-	-	0/2/2/2	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	38	DMF	O-C-N-C2
3	C	38	DMF	O-C-N-C1
3	R	34	DMF	O-C-N-C2
3	R	34	DMF	O-C-N-C1
3	C	55	DMF	O-C-N-C1

There are no ring outliers.

15 monomers are involved in 33 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	K	250	DMF	1	0
3	N	22	DMF	1	0
3	V	27	DMF	1	0
3	X	40	DMF	1	0
3	R	34	DMF	2	0
3	Z	18	DMF	2	0
3	E	66	DMF	3	0
3	L	53	DMF	2	0
3	C	10	DMF	1	0
3	J	4	DMF	5	0
3	C	55	DMF	5	0
3	M	249	DMF	2	0
3	G	12	DMF	2	0
3	P	14	DMF	1	0
3	T	29	DMF	4	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^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	1	215/248 (86%)	0.93	32 (14%)	7	6	19, 54, 89, 99	0
1	A	215/248 (86%)	0.95	30 (13%)	7	7	18, 54, 91, 98	0
1	B	214/248 (86%)	1.05	44 (20%)	3	3	19, 55, 89, 97	0
1	D	214/248 (86%)	1.06	34 (15%)	6	6	17, 55, 91, 98	0
1	F	216/248 (87%)	0.91	39 (18%)	4	4	19, 55, 87, 95	0
1	I	214/248 (86%)	0.95	33 (15%)	6	6	18, 54, 88, 94	0
1	K	215/248 (86%)	1.04	38 (17%)	4	5	18, 56, 89, 98	0
1	M	215/248 (86%)	1.03	38 (17%)	4	5	19, 53, 88, 98	0
1	O	215/248 (86%)	0.92	30 (13%)	7	7	19, 53, 89, 94	0
1	Q	217/248 (87%)	1.05	42 (19%)	4	4	18, 53, 87, 95	0
1	S	215/248 (86%)	0.93	31 (14%)	7	7	18, 55, 93, 100	0
1	U	214/248 (86%)	0.95	35 (16%)	5	5	18, 54, 91, 96	0
1	W	217/248 (87%)	1.04	33 (15%)	6	6	20, 55, 92, 97	0
1	Y	213/248 (85%)	1.29	55 (25%)	2	2	20, 56, 94, 105	0
2	2	214/240 (89%)	-0.31	5 (2%)	61	58	4, 20, 45, 67	0
2	C	214/240 (89%)	-0.29	5 (2%)	61	58	6, 20, 48, 73	0
2	E	215/240 (89%)	-0.35	3 (1%)	73	70	6, 20, 47, 72	0
2	G	215/240 (89%)	-0.29	3 (1%)	73	70	8, 22, 48, 74	0
2	H	212/240 (88%)	-0.33	3 (1%)	73	70	8, 21, 44, 64	0
2	J	215/240 (89%)	-0.30	5 (2%)	61	58	7, 20, 48, 64	0
2	L	215/240 (89%)	-0.26	5 (2%)	61	58	5, 21, 48, 71	0
2	N	212/240 (88%)	-0.33	2 (0%)	81	78	4, 20, 44, 64	0
2	P	215/240 (89%)	-0.31	3 (1%)	73	70	6, 22, 49, 72	0
2	R	222/240 (92%)	-0.36	7 (3%)	50	47	7, 20, 48, 67	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å^2)	Q<0.9
2	T	215/240 (89%)	-0.28	6 (2%)	55 51	8, 22, 49, 77	0
2	V	221/240 (92%)	-0.41	4 (1%)	67 64	3, 20, 44, 69	0
2	X	215/240 (89%)	-0.31	6 (2%)	55 51	8, 22, 49, 75	0
2	Z	214/240 (89%)	-0.29	2 (0%)	81 78	9, 23, 48, 64	0
All	All	6023/6832 (88%)	0.34	573 (9%)	15 14	3, 34, 86, 105	0

The worst 5 of 573 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	1	9	PRO	7.0
1	M	7	ILE	6.3
1	B	234	LEU	5.5
1	Y	233	LEU	4.9
1	W	7	ILE	4.8

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
2	OZT	L	301	9/10	0.93	0.08	19,24,26,27	0
2	OZT	X	301	9/10	0.93	0.08	19,21,23,26	0
2	OZT	J	301	9/10	0.94	0.07	19,23,27,31	0
2	OZT	G	301	9/10	0.94	0.07	21,24,29,32	0
2	OZT	P	301	9/10	0.94	0.07	23,28,30,33	0
2	OZT	V	301	9/10	0.94	0.08	20,22,27,31	0
2	OZT	H	301	9/10	0.94	0.08	22,24,25,28	0
2	OZT	R	301	9/10	0.95	0.07	20,23,27,28	0
2	OZT	2	301	9/10	0.95	0.08	25,31,33,35	0
2	OZT	N	301	9/10	0.96	0.06	21,24,27,31	0
2	OZT	Z	301	9/10	0.96	0.06	19,21,23,24	0
2	OZT	C	301	9/10	0.96	0.06	18,23,26,29	0
2	OZT	T	301	9/10	0.97	0.05	22,22,24,25	0
2	OZT	E	301	9/10	0.98	0.04	20,23,25,27	0

6.3 Carbohydrates (i)

There are no monosaccharides 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, 95^{th} 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	H	32	5/5	0.45	0.29	73,74,75,76	0
3	DMF	X	40	5/5	0.55	0.34	92,93,93,93	0
3	DMF	P	51	5/5	0.60	0.31	76,76,76,76	0
3	DMF	1	250	5/5	0.68	0.31	61,62,63,63	0
3	DMF	2	49	5/5	0.69	0.43	93,93,94,94	0
3	DMF	P	14	5/5	0.70	0.42	90,91,92,92	0
3	DMF	V	39	5/5	0.71	0.28	72,72,72,72	0
3	DMF	G	64	5/5	0.71	0.29	56,57,58,58	0
3	DMF	J	45	5/5	0.73	0.36	85,85,85,85	0
3	DMF	E	20	5/5	0.74	0.34	84,84,85,85	0
3	DMF	K	250	5/5	0.74	0.24	57,59,59,60	0
3	DMF	E	66	5/5	0.75	0.28	65,65,66,67	0
3	DMF	Z	41	5/5	0.75	0.34	93,93,93,93	0
3	DMF	G	12	5/5	0.76	0.24	66,67,67,67	0
3	DMF	Z	54	5/5	0.77	0.34	85,86,86,86	0
3	DMF	N	58	5/5	0.77	0.25	54,56,58,59	0
3	DMF	C	47	5/5	0.77	0.27	71,71,71,72	0
3	DMF	J	4	5/5	0.78	0.21	60,61,61,62	0
3	DMF	C	38	5/5	0.78	0.23	63,64,64,65	0
3	DMF	R	59	5/5	0.78	0.25	58,59,60,60	0
3	DMF	K	251	5/5	0.79	0.20	60,62,62,62	0
3	DMF	M	250	5/5	0.79	0.16	39,40,41,41	0
3	DMF	I	249	5/5	0.80	0.23	55,56,58,59	0
3	DMF	N	22	5/5	0.80	0.35	91,92,92,92	0
3	DMF	2	52	5/5	0.80	0.27	75,75,76,76	0
3	DMF	B	249	5/5	0.81	0.17	47,47,48,48	0
3	DMF	H	26	5/5	0.82	0.23	64,64,65,65	0
3	DMF	D	249	5/5	0.82	0.18	53,53,53,54	0
3	DMF	L	53	5/5	0.83	0.27	84,84,85,86	0
3	DMF	C	10	5/5	0.83	0.17	42,45,46,48	0
3	DMF	N	2	5/5	0.83	0.23	69,69,70,70	0
3	DMF	G	24	5/5	0.83	0.29	80,80,81,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	DMF	L	3	5/5	0.83	0.22	57,58,59,60	0
3	DMF	C	55	5/5	0.85	0.23	74,74,74,74	0
3	DMF	F	249	5/5	0.85	0.22	70,71,71,71	0
3	DMF	P	56	5/5	0.85	0.24	64,64,64,65	0
3	DMF	X	61	5/5	0.85	0.17	55,56,58,60	0
3	DMF	Z	18	5/5	0.85	0.35	97,98,98,99	0
3	DMF	B	250	5/5	0.86	0.23	77,78,78,79	0
3	DMF	T	67	5/5	0.86	0.21	51,51,53,53	0
3	DMF	1	249	5/5	0.86	0.16	49,51,51,52	0
3	DMF	P	65	5/5	0.87	0.17	50,51,52,52	0
3	DMF	W	249	5/5	0.88	0.29	76,76,77,78	0
3	DMF	G	60	5/5	0.88	0.18	50,52,52,52	0
3	DMF	Z	43	5/5	0.89	0.17	48,48,49,49	0
3	DMF	R	34	5/5	0.89	0.22	68,69,70,71	0
3	DMF	M	249	5/5	0.89	0.15	54,54,55,56	0
3	DMF	T	29	5/5	0.89	0.18	63,63,63,63	0
3	DMF	O	249	5/5	0.89	0.16	46,47,48,50	0
3	DMF	H	62	5/5	0.89	0.17	42,43,45,47	0
3	DMF	N	15	5/5	0.90	0.13	44,46,47,47	0
3	DMF	Z	30	5/5	0.90	0.16	56,56,57,57	0
3	DMF	Q	249	5/5	0.90	0.13	49,49,50,50	0
3	DMF	G	1	5/5	0.91	0.14	42,44,45,46	0
3	DMF	H	33	5/5	0.91	0.14	39,40,41,41	0
3	DMF	X	16	5/5	0.91	0.14	46,46,47,48	0
3	DMF	E	28	5/5	0.91	0.16	45,47,48,48	0
3	DMF	S	249	5/5	0.91	0.23	79,80,81,81	0
3	DMF	J	50	5/5	0.91	0.16	57,58,58,58	0
3	DMF	K	249	5/5	0.91	0.14	51,53,54,55	0
3	DMF	U	249	5/5	0.92	0.15	51,51,52,52	0
3	DMF	V	27	5/5	0.92	0.27	77,77,78,79	0
3	DMF	2	42	5/5	0.92	0.17	54,54,55,55	0
3	DMF	A	249	5/5	0.92	0.17	60,61,62,62	0
3	DMF	L	36	5/5	0.92	0.14	57,57,58,58	0
3	DMF	2	63	5/5	0.92	0.12	43,45,45,46	0
3	DMF	I	250	5/5	0.93	0.14	61,61,61,61	0

6.5 Other polymers (i)

There are no such residues in this entry.