



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 15, 2020 – 02:57 pm BST

PDB ID : 3H6I  
Title : Crystal Structure of Mycobacterium Tuberculosis Proteasome Modified by inhibitor GL1  
Authors : Li, D.; Li, H.; Lin, G.  
Deposited on : 2009-04-23  
Resolution : 2.43 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

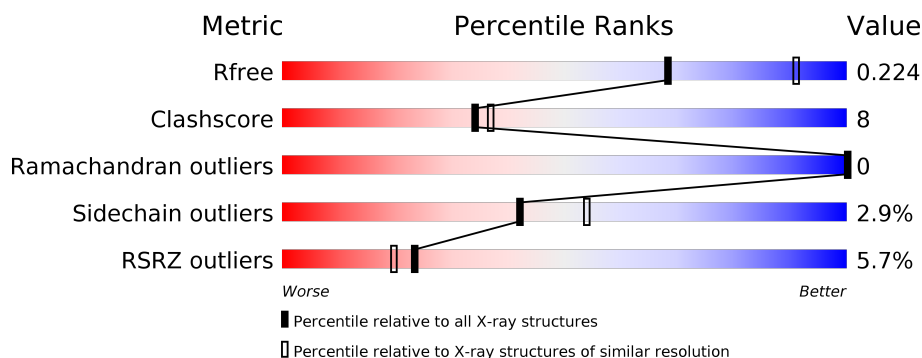
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.43 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.



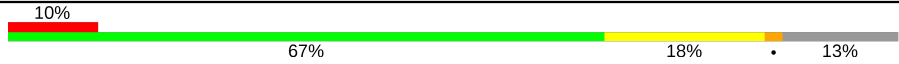



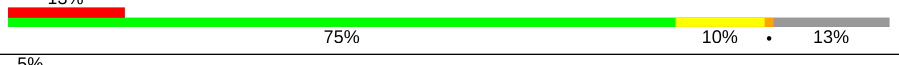
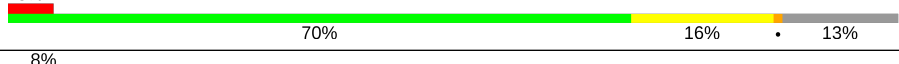
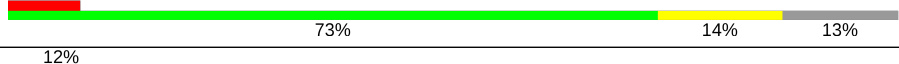

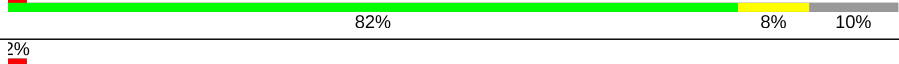


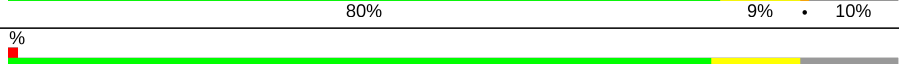

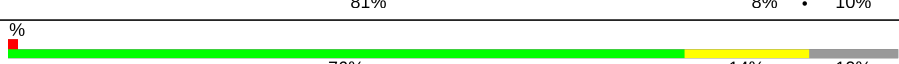

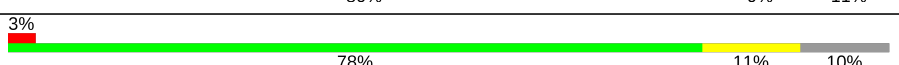
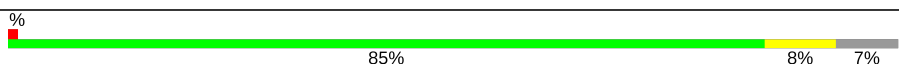
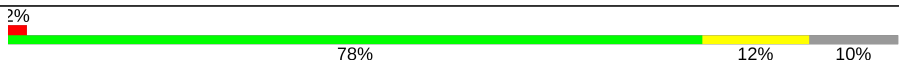
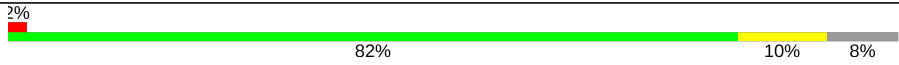



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1564 (2.46-2.42)
Clashscore	141614	1631 (2.46-2.42)
Ramachandran outliers	138981	1617 (2.46-2.42)
Sidechain outliers	138945	1617 (2.46-2.42)
RSRZ outliers	127900	1547 (2.46-2.42)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	1	248	<div> <div>8%</div> <div> <div></div> <div>75%</div> <div>10%</div> <div>•</div> <div>13%</div> </div> </div>
1	A	248	<div> <div>14%</div> <div> <div></div> <div>75%</div> <div>11%</div> <div>13%</div> </div> </div>
1	B	248	<div> <div>6%</div> <div> <div></div> <div>74%</div> <div>12%</div> <div>•</div> <div>14%</div> </div> </div>
1	D	248	<div> <div>11%</div> <div> <div></div> <div>71%</div> <div>12%</div> <div>•</div> <div>14%</div> </div> </div>
1	F	248	<div> <div>6%</div> <div> <div></div> <div>73%</div> <div>14%</div> <div>•</div> <div>13%</div> </div> </div>
1	I	248	<div> <div>8%</div> <div> <div></div> <div>75%</div> <div>12%</div> <div>13%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	K	248	
1	M	248	
1	O	248	
1	Q	248	
1	S	248	
1	U	248	
1	W	248	
1	Y	248	
2	2	240	
2	C	240	
2	E	240	
2	G	240	
2	H	240	
2	J	240	
2	L	240	
2	N	240	
2	P	240	
2	R	240	
2	T	240	
2	V	240	
2	X	240	
2	Z	240	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	OZT	P	301	-	-	X	-
3	DMF	C	5	-	-	X	-
3	DMF	C	64	-	-	X	-
3	DMF	C	73	-	-	X	-
3	DMF	D	249	-	-	-	X
3	DMF	E	32	-	-	-	X
3	DMF	H	19	-	-	X	-
3	DMF	H	31	-	-	-	X
3	DMF	J	6	-	-	X	-
3	DMF	O	250	-	-	X	-
3	DMF	T	35	-	-	X	-
3	DMF	T	94	-	-	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 48540 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	216	Total	C	N	O	S	0	0	0
			1662	1041	304	314	3			
1	B	214	Total	C	N	O	S	0	0	0
			1650	1033	302	312	3			
1	D	213	Total	C	N	O	S	0	0	0
			1644	1030	301	310	3			
1	F	217	Total	C	N	O	S	0	0	0
			1669	1045	305	316	3			
1	I	215	Total	C	N	O	S	0	0	0
			1656	1038	303	312	3			
1	K	217	Total	C	N	O	S	0	0	0
			1670	1047	305	315	3			
1	M	216	Total	C	N	O	S	0	0	0
			1662	1041	304	314	3			
1	O	215	Total	C	N	O	S	0	0	0
			1654	1035	303	313	3			
1	Q	218	Total	C	N	O	S	0	0	0
			1677	1051	306	317	3			
1	S	215	Total	C	N	O	S	0	0	0
			1654	1035	303	313	3			
1	U	215	Total	C	N	O	S	0	0	0
			1654	1035	303	313	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 1593	C 998	N 274	O 317	S 4	0	0	0
2	E	216	Total 1601	C 1004	N 275	O 318	S 4	0	0	0
2	G	216	Total 1601	C 1004	N 275	O 318	S 4	0	0	0
2	H	213	Total 1583	C 992	N 272	O 315	S 4	0	0	0
2	J	216	Total 1601	C 1004	N 275	O 318	S 4	0	0	0
2	L	216	Total 1601	C 1004	N 275	O 318	S 4	0	0	0
2	N	213	Total 1580	C 989	N 272	O 315	S 4	0	0	0
2	P	216	Total 1601	C 1004	N 275	O 318	S 4	0	0	0
2	R	223	Total 1646	C 1031	N 282	O 329	S 4	0	0	0
2	T	216	Total 1601	C 1004	N 275	O 318	S 4	0	0	0
2	V	221	Total 1632	C 1022	N 280	O 326	S 4	0	0	0
2	X	216	Total 1601	C 1004	N 275	O 318	S 4	0	0	0
2	Z	215	Total 1593	C 998	N 274	O 317	S 4	0	0	0
2	2	215	Total 1593	C 998	N 274	O 317	S 4	0	0	0

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

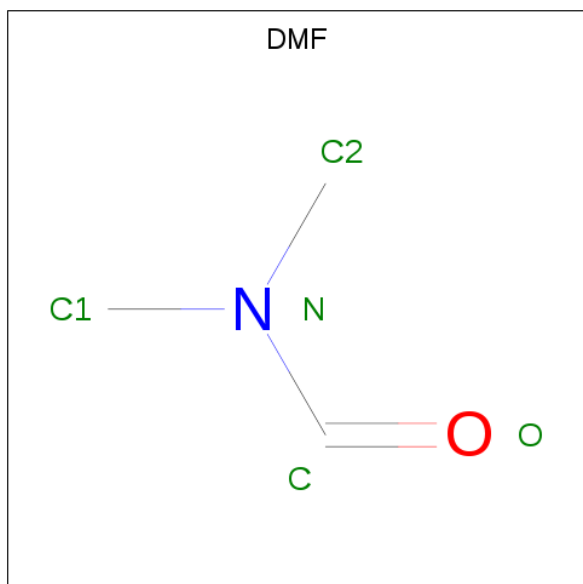
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Chain	Residue	Modelled	Actual	Comment	Reference
2	539	HIS	-	EXPRESSION TAG	UNP O33245
2	540	HIS	-	EXPRESSION TAG	UNP O33245

- Molecule 3 is DIMETHYLFORMAMIDE (three-letter code: 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	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	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		

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

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	H	1	Total 5	C 3	N 1	O 1	0	0
3	H	1	Total 5	C 3	N 1	O 1	0	0
3	H	1	Total 5	C 3	N 1	O 1	0	0
3	H	1	Total 5	C 3	N 1	O 1	0	0
3	H	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	I	1	Total 5	C 3	N 1	O 1	0	0
3	J	1	Total 5	C 3	N 1	O 1	0	0
3	J	1	Total 5	C 3	N 1	O 1	0	0
3	J	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	L	1	Total 5	C 3	N 1	O 1	0	0
3	L	1	Total 5	C 3	N 1	O 1	0	0
3	L	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	M	1	Total 5	C 3	N 1	O 1	0	0
3	N	1	Total 5	C 3	N 1	O 1	0	0
3	N	1	Total 5	C 3	N 1	O 1	0	0
3	N	1	Total 5	C 3	N 1	O 1	0	0
3	N	1	Total 5	C 3	N 1	O 1	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	N	1	Total 5	C 3	N 1	O 1	0	0
3	N	1	Total 5	C 3	N 1	O 1	0	0
3	N	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	O	1	Total 5	C 3	N 1	O 1	0	0
3	P	1	Total 5	C 3	N 1	O 1	0	0
3	P	1	Total 5	C 3	N 1	O 1	0	0
3	P	1	Total 5	C 3	N 1	O 1	0	0
3	P	1	Total 5	C 3	N 1	O 1	0	0
3	P	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	R	1	Total 5	C 3	N 1	O 1	0	0
3	R	1	Total 5	C 3	N 1	O 1	0	0
3	R	1	Total 5	C 3	N 1	O 1	0	0
3	R	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	S	1	Total 5	C 3	N 1	O 1	0	0
3	T	1	Total 5	C 3	N 1	O 1	0	0
3	T	1	Total 5	C 3	N 1	O 1	0	0

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

*Continued on next page...*

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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	43	Total	O	0	0
			43	43		
4	B	45	Total	O	0	0
			45	45		
4	C	142	Total	O	0	0
			142	142		
4	D	43	Total	O	0	0
			43	43		
4	E	124	Total	O	0	0
			124	124		
4	F	34	Total	O	0	0
			34	34		
4	G	136	Total	O	0	0
			136	136		
4	H	122	Total	O	0	0
			122	122		
4	I	37	Total	O	0	0
			37	37		
4	J	128	Total	O	0	0
			128	128		
4	K	45	Total	O	0	0
			45	45		

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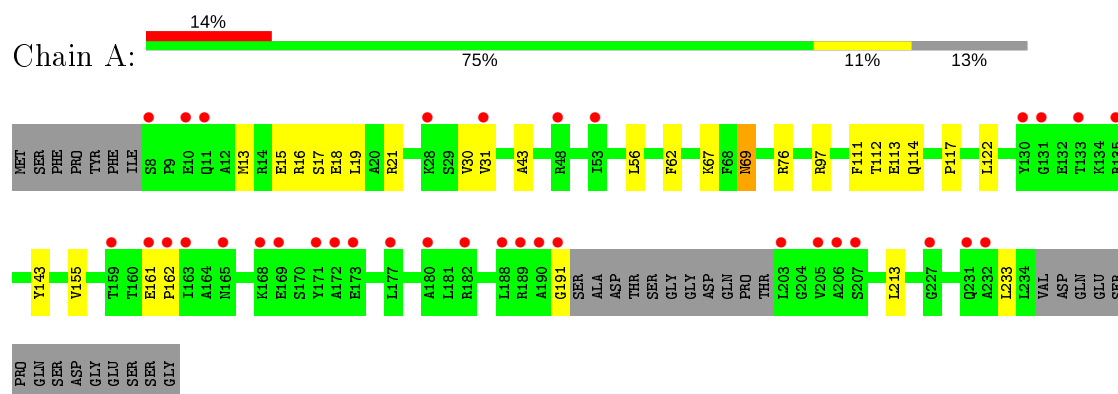
*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	L	138	Total 138	O 138	0	0
4	M	52	Total 52	O 52	0	0
4	N	118	Total 118	O 118	0	0
4	O	51	Total 51	O 51	0	0
4	P	111	Total 111	O 111	0	0
4	Q	41	Total 41	O 41	0	0
4	R	141	Total 141	O 141	0	0
4	S	31	Total 31	O 31	0	0
4	T	112	Total 112	O 112	0	0
4	U	43	Total 43	O 43	0	0
4	V	154	Total 154	O 154	0	0
4	W	31	Total 31	O 31	0	0
4	X	130	Total 130	O 130	0	0
4	Y	41	Total 41	O 41	0	0
4	Z	113	Total 113	O 113	0	0
4	1	42	Total 42	O 42	0	0
4	2	133	Total 133	O 133	0	0

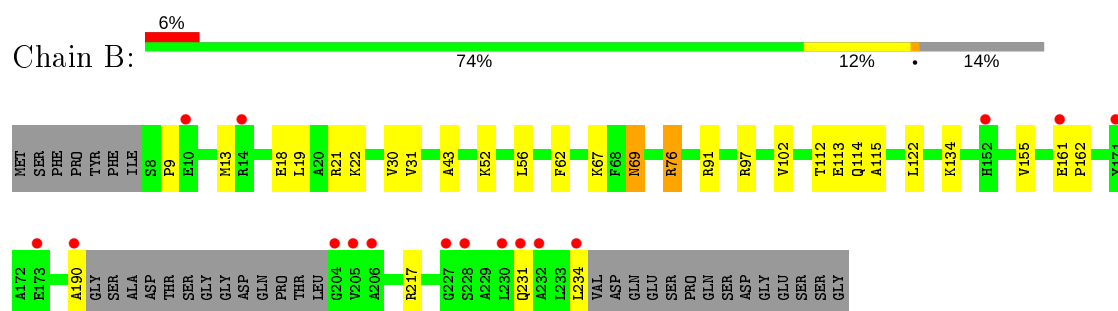
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

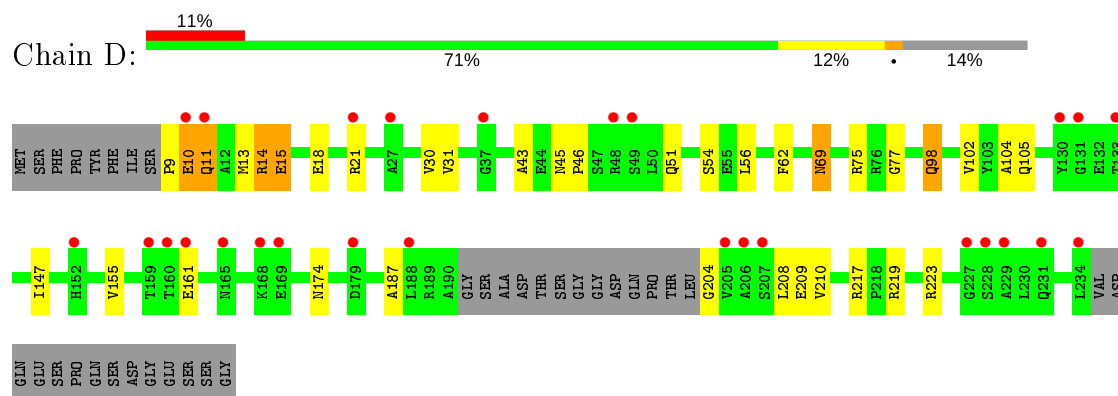
#### • Molecule 1: Proteasome (Alpha subunit) PrcA



#### • Molecule 1: Proteasome (Alpha subunit) PrcA

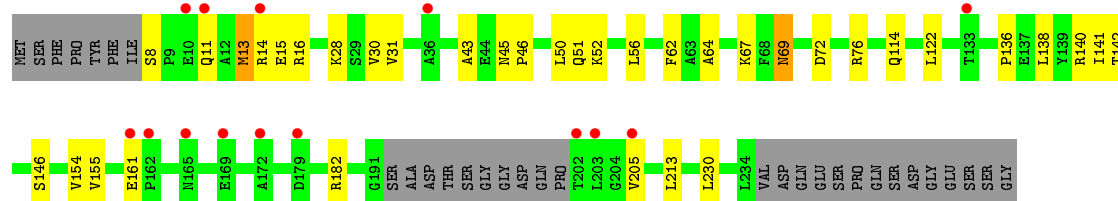


#### • Molecule 1: Proteasome (Alpha subunit) PrcA

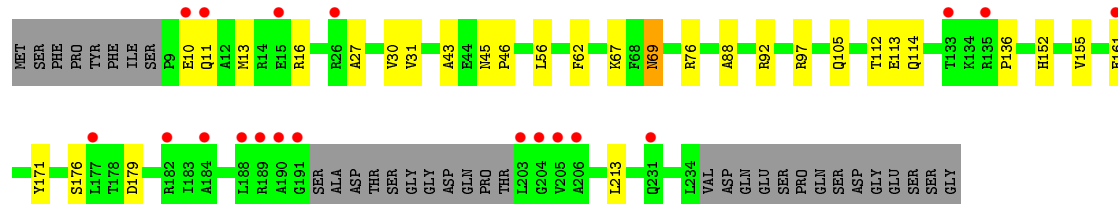
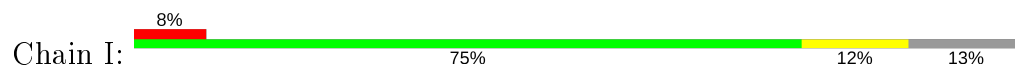


#### • Molecule 1: Proteasome (Alpha subunit) PrcA

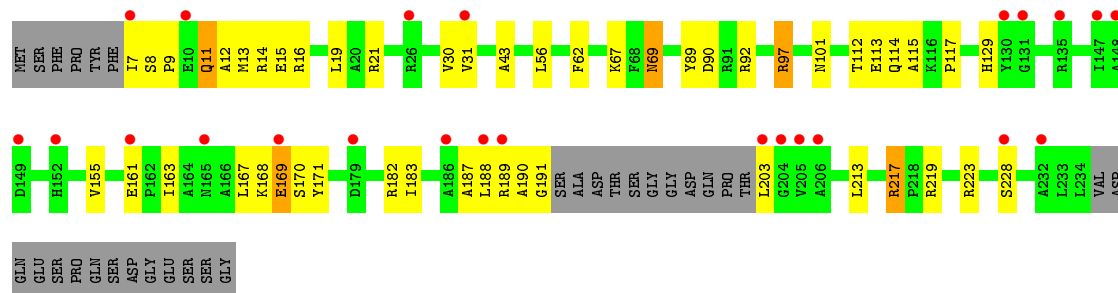




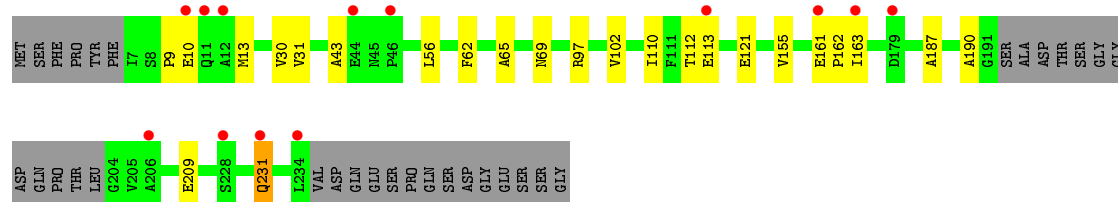
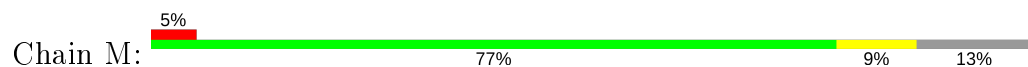
- Molecule 1: Proteasome (Alpha subunit) PrcA



- Molecule 1: Proteasome (Alpha subunit) PrcA

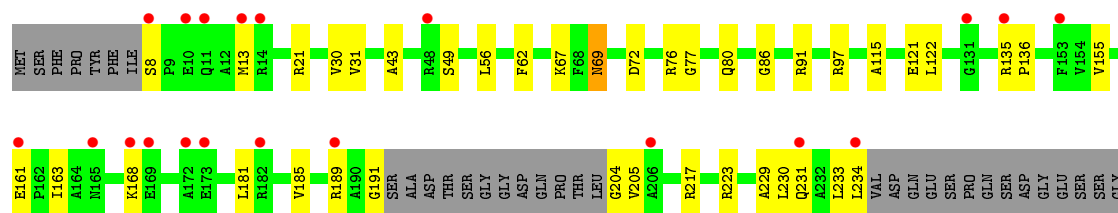


- Molecule 1: Proteasome (Alpha subunit) PrcA

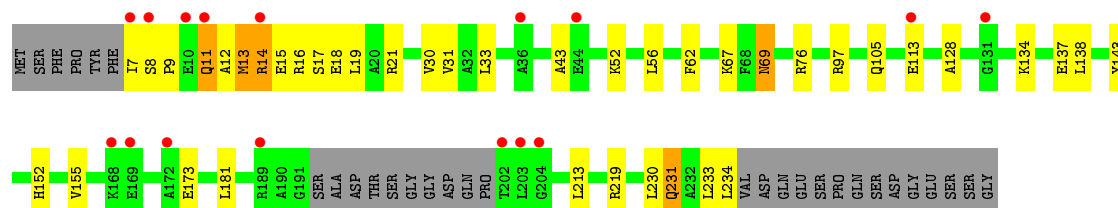


- Molecule 1: Proteasome (Alpha subunit) PrcA

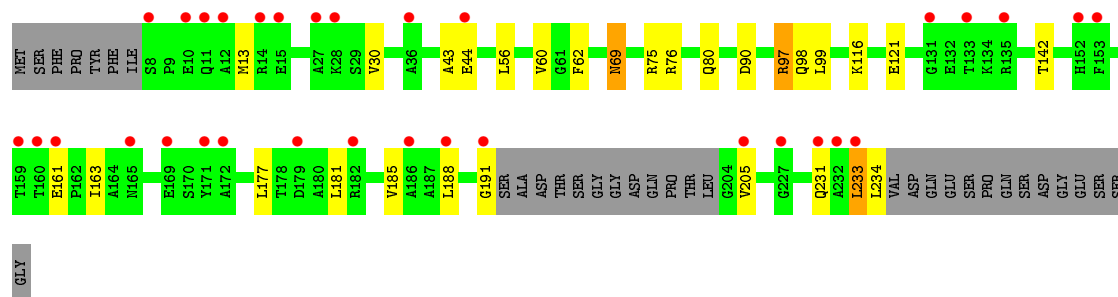
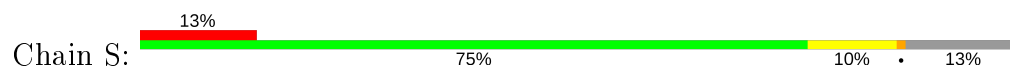




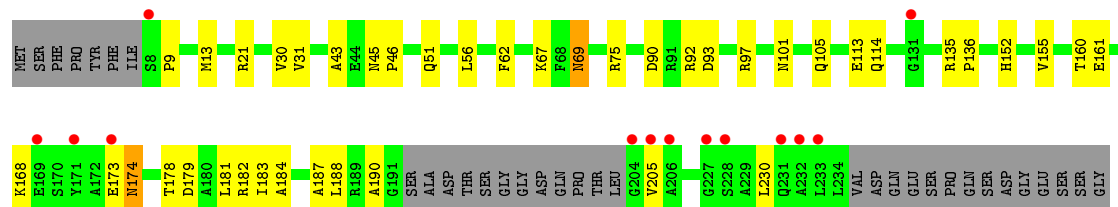
• Molecule 1: Proteasome (Alpha subunit) PrcA



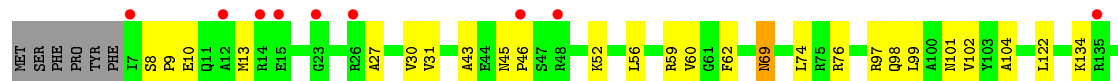
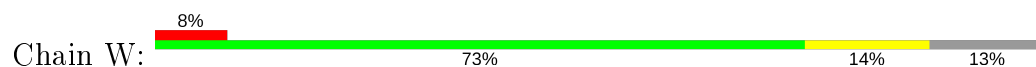
• Molecule 1: Proteasome (Alpha subunit) PrcA

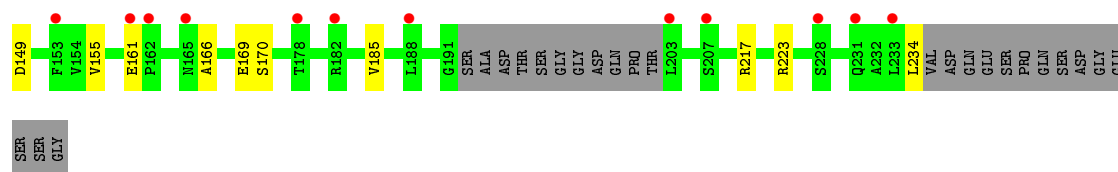


• Molecule 1: Proteasome (Alpha subunit) PrcA

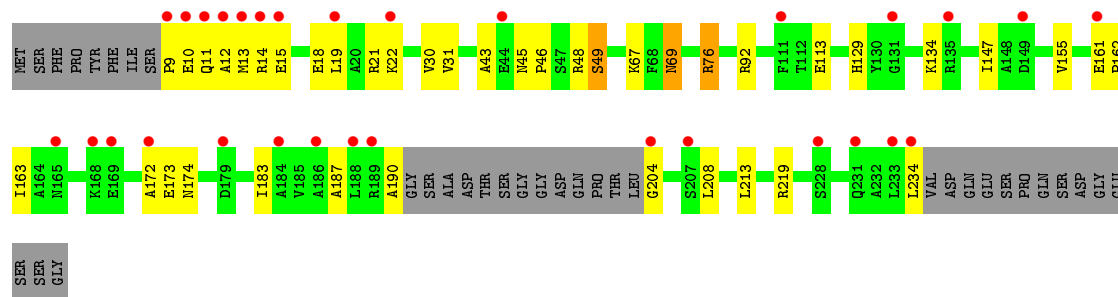


• Molecule 1: Proteasome (Alpha subunit) PrcA

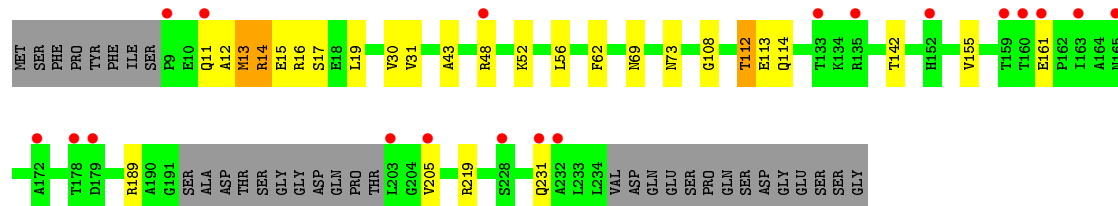




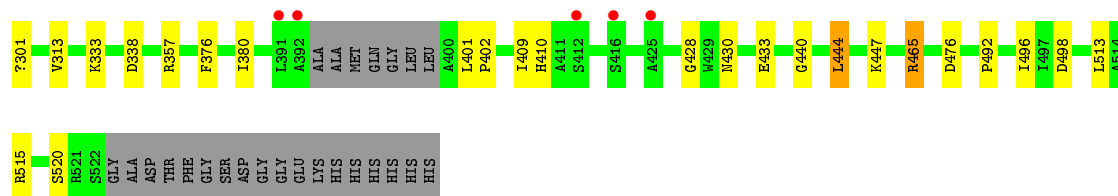
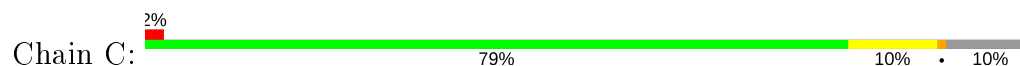
- Molecule 1: Proteasome (Alpha subunit) PrcA



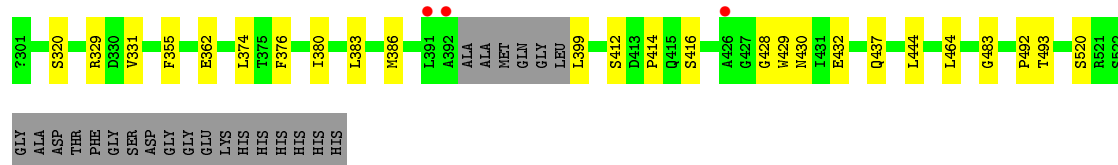
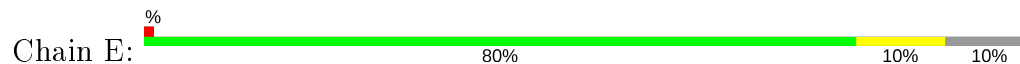
- Molecule 1: Proteasome (Alpha subunit) PrcA




- Molecule 2: Proteasome (Beta subunit) PrcB

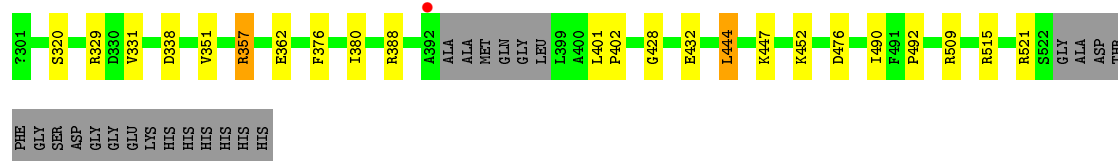


- Molecule 2: Proteasome (Beta subunit) PrcB




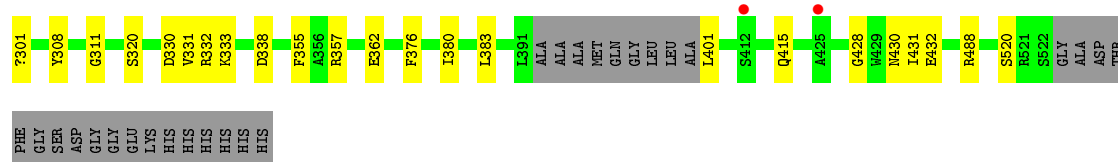
- Molecule 2: Proteasome (Beta subunit) PrcB

Chain G: 




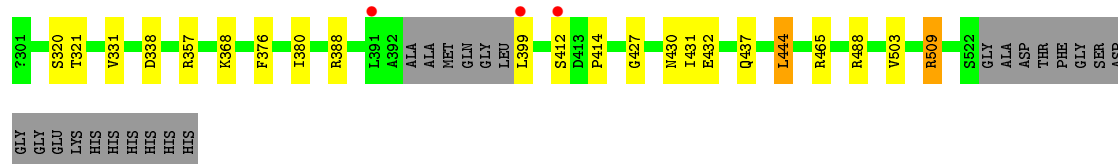
- Molecule 2: Proteasome (Beta subunit) PrcB

Chain H: 




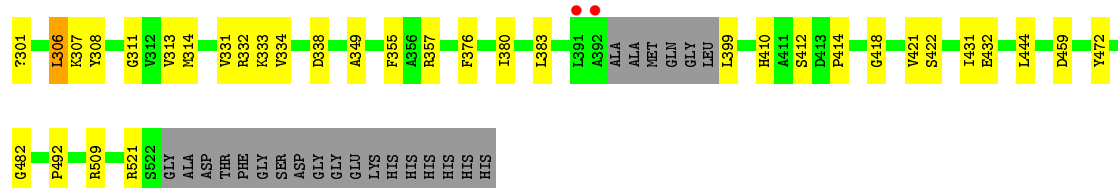
- Molecule 2: Proteasome (Beta subunit) PrcB

Chain J: 




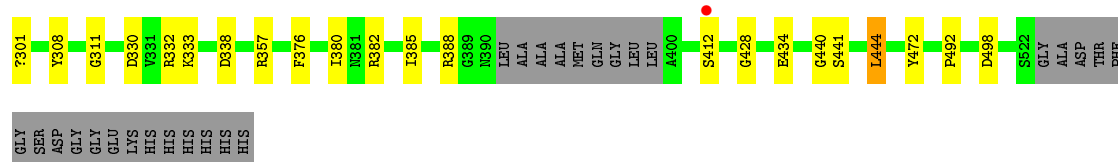
- Molecule 2: Proteasome (Beta subunit) PrcB

Chain L: 

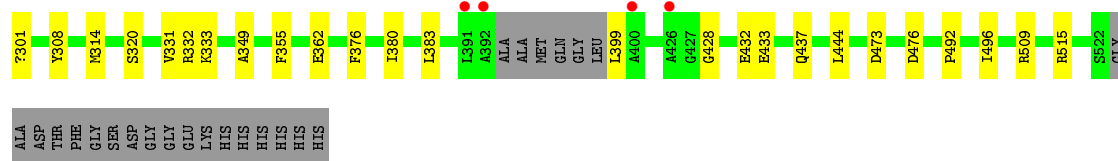
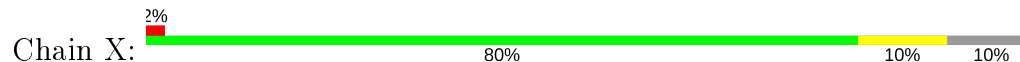
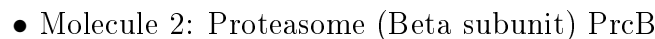
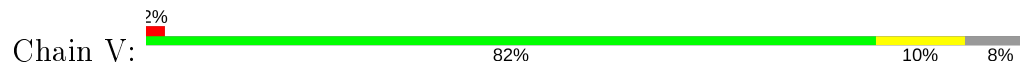
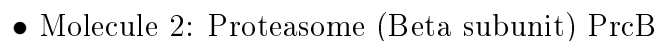
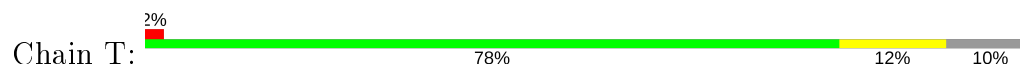
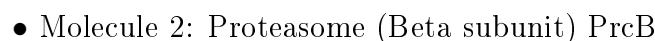
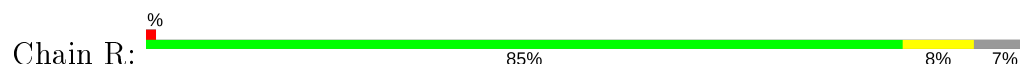
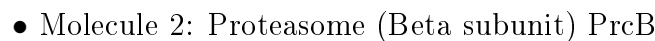


- Molecule 2: Proteasome (Beta subunit) PrcB

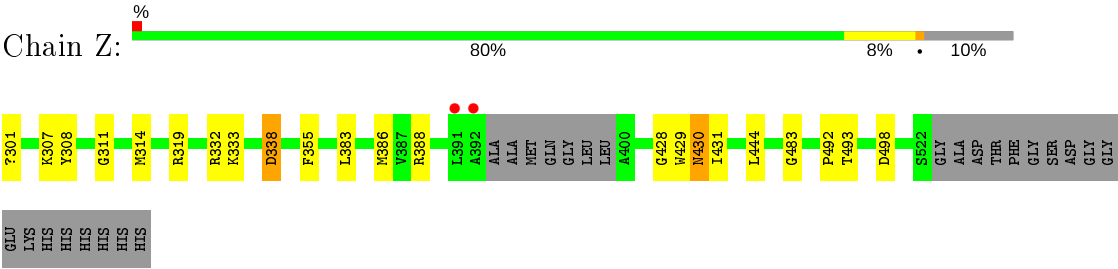
Chain N: 



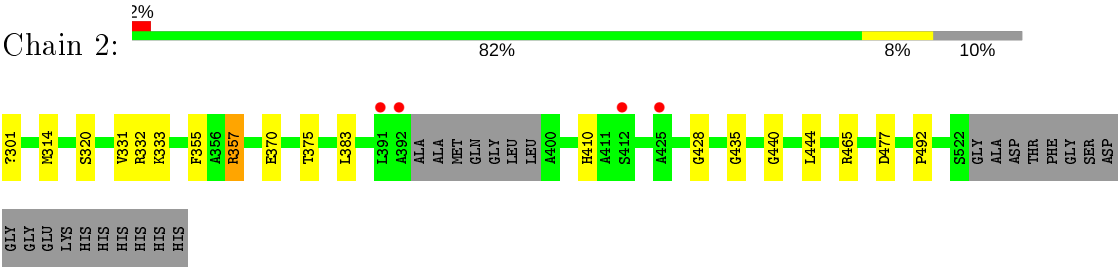
Chain P: 



● Molecule 2: Proteasome (Beta subunit) PrcB



● Molecule 2: Proteasome (Beta subunit) PrcB



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	171.62Å 117.67Å 196.34Å 90.00° 113.65° 90.00°	Depositor
Resolution (Å)	29.75 – 2.43 30.57 – 2.44	Depositor EDS
% Data completeness (in resolution range)	97.8 (29.75-2.43) 97.9 (30.57-2.44)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.82 (at 2.45Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.204 , 0.232 0.196 , 0.224	Depositor DCC
$R_{free}$ test set	13191 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	30.5	Xtriage
Anisotropy	0.198	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 48.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.003 for h,-k,-h-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	48540	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.73% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 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: 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	0.76	0/1681	0.85	0/2270
1	A	0.75	0/1687	0.83	1/2279 (0.0%)
1	B	0.76	0/1675	0.85	2/2263 (0.1%)
1	D	0.75	0/1669	0.84	1/2254 (0.0%)
1	F	0.76	0/1694	0.84	1/2289 (0.0%)
1	I	0.73	0/1681	0.87	2/2270 (0.1%)
1	K	0.74	0/1695	0.85	2/2290 (0.1%)
1	M	0.77	0/1687	0.86	0/2279
1	O	0.78	0/1679	0.84	1/2268 (0.0%)
1	Q	0.76	0/1702	0.81	2/2300 (0.1%)
1	S	0.74	0/1679	0.85	1/2268 (0.0%)
1	U	0.77	0/1679	0.85	2/2268 (0.1%)
1	W	0.76	0/1695	0.86	0/2290
1	Y	0.75	0/1669	0.85	2/2254 (0.1%)
2	2	0.89	1/1607 (0.1%)	0.84	1/2178 (0.0%)
2	C	0.87	1/1607 (0.1%)	0.88	2/2178 (0.1%)
2	E	0.91	0/1615	0.88	0/2189
2	G	0.89	0/1615	0.88	3/2189 (0.1%)
2	H	0.91	0/1597	0.87	2/2164 (0.1%)
2	J	0.92	1/1615 (0.1%)	0.87	1/2189 (0.0%)
2	L	0.91	0/1615	0.87	0/2189
2	N	0.89	0/1594	0.87	1/2160 (0.0%)
2	P	0.86	1/1615 (0.1%)	0.85	1/2189 (0.0%)
2	R	0.88	0/1661	0.86	0/2251
2	T	0.86	0/1615	0.86	1/2189 (0.0%)
2	V	0.92	0/1647	0.83	0/2232
2	X	0.91	1/1615 (0.1%)	0.88	1/2189 (0.0%)
2	Z	0.88	1/1607 (0.1%)	0.87	2/2178 (0.1%)
All	All	0.83	6/46197 (0.0%)	0.86	32/62506 (0.1%)

The worst 5 of 6 bond length outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	313	VAL	CB-CG1	-5.88	1.40	1.52
2	2	314	MET	SD-CE	-5.82	1.45	1.77
2	J	503	VAL	CA-CB	5.34	1.66	1.54
2	P	496	ILE	C-N	-5.29	1.21	1.34
2	X	308	TYR	CD2-CE2	5.19	1.47	1.39

The worst 5 of 32 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	465	ARG	NE-CZ-NH2	-5.67	117.47	120.30
2	H	357	ARG	NE-CZ-NH1	5.61	123.11	120.30
1	A	122	LEU	CA-CB-CG	5.61	128.20	115.30
1	K	21	ARG	NE-CZ-NH1	5.57	123.08	120.30
1	B	76	ARG	NE-CZ-NH2	-5.51	117.55	120.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	1656	0	1658	32	0
1	A	1662	0	1662	29	0
1	B	1650	0	1648	32	0
1	D	1644	0	1644	33	0
1	F	1669	0	1669	38	0
1	I	1656	0	1658	24	0
1	K	1670	0	1673	51	0
1	M	1662	0	1662	16	0
1	O	1654	0	1651	44	0
1	Q	1677	0	1680	38	0
1	S	1654	0	1651	20	0
1	U	1654	0	1651	37	0
1	W	1670	0	1673	27	0
1	Y	1644	0	1644	48	0
2	2	1593	0	1577	19	0
2	C	1593	0	1577	32	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	1601	0	1588	19	0
2	G	1601	0	1588	23	0
2	H	1583	0	1567	17	0
2	J	1601	0	1588	24	0
2	L	1601	0	1588	31	0
2	N	1580	0	1561	19	0
2	P	1601	0	1587	24	0
2	R	1646	0	1624	23	0
2	T	1601	0	1588	25	0
2	V	1632	0	1608	15	0
2	X	1601	0	1588	17	0
2	Z	1593	0	1577	17	0
3	1	15	0	21	3	0
3	2	15	0	21	1	0
3	A	10	0	14	2	0
3	B	15	0	21	2	0
3	C	40	0	56	20	0
3	D	20	0	28	2	0
3	E	30	0	42	5	0
3	F	10	0	14	1	0
3	G	20	0	28	8	0
3	H	35	0	49	8	0
3	I	10	0	14	0	0
3	J	15	0	21	5	0
3	K	10	0	14	2	0
3	L	15	0	21	5	0
3	M	10	0	14	1	0
3	N	35	0	49	7	0
3	O	10	0	14	6	0
3	P	25	0	35	2	0
3	Q	10	0	14	0	0
3	R	20	0	28	2	0
3	S	15	0	21	1	0
3	T	25	0	35	9	0
3	U	20	0	28	4	0
3	V	20	0	28	1	0
3	W	10	0	14	1	0
3	X	15	0	21	1	0
3	Y	5	0	7	0	0
3	Z	30	0	42	10	0
4	1	42	0	0	9	0
4	2	133	0	0	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	43	0	0	5	0
4	B	45	0	0	13	0
4	C	142	0	0	12	0
4	D	43	0	0	15	0
4	E	124	0	0	8	0
4	F	34	0	0	6	0
4	G	136	0	0	18	0
4	H	122	0	0	13	0
4	I	37	0	0	9	0
4	J	128	0	0	16	0
4	K	45	0	0	17	0
4	L	138	0	0	7	0
4	M	52	0	0	6	0
4	N	118	0	0	10	0
4	O	51	0	0	17	0
4	P	111	0	0	10	0
4	Q	41	0	0	4	0
4	R	141	0	0	14	0
4	S	31	0	0	5	0
4	T	112	0	0	9	0
4	U	43	0	0	13	0
4	V	154	0	0	8	0
4	W	31	0	0	5	0
4	X	130	0	0	5	0
4	Y	41	0	0	21	0
4	Z	113	0	0	17	0
All	All	48540	0	46144	775	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 8.

The worst 5 of 775 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:V:400:ALA:HA	4:V:2033:HOH:O	1.27	1.32
2:C:430:ASN:HB2	4:C:2190:HOH:O	1.33	1.26
2:C:447:LYS:CD	3:C:5:DMF:H12	1.66	1.26
2:V:332:ARG:HB3	4:V:2317:HOH:O	1.32	1.25
1:U:160:THR:HG22	4:U:2365:HOH:O	1.34	1.24

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	1	211/248 (85%)	206 (98%)	5 (2%)	0	100	100
1	A	212/248 (86%)	207 (98%)	5 (2%)	0	100	100
1	B	210/248 (85%)	206 (98%)	4 (2%)	0	100	100
1	D	209/248 (84%)	205 (98%)	4 (2%)	0	100	100
1	F	213/248 (86%)	209 (98%)	4 (2%)	0	100	100
1	I	211/248 (85%)	207 (98%)	4 (2%)	0	100	100
1	K	213/248 (86%)	208 (98%)	5 (2%)	0	100	100
1	M	212/248 (86%)	206 (97%)	6 (3%)	0	100	100
1	O	211/248 (85%)	208 (99%)	3 (1%)	0	100	100
1	Q	214/248 (86%)	207 (97%)	7 (3%)	0	100	100
1	S	211/248 (85%)	208 (99%)	3 (1%)	0	100	100
1	U	211/248 (85%)	208 (99%)	3 (1%)	0	100	100
1	W	213/248 (86%)	209 (98%)	4 (2%)	0	100	100
1	Y	209/248 (84%)	205 (98%)	4 (2%)	0	100	100
2	2	211/240 (88%)	210 (100%)	1 (0%)	0	100	100
2	C	211/240 (88%)	210 (100%)	1 (0%)	0	100	100
2	E	212/240 (88%)	211 (100%)	1 (0%)	0	100	100
2	G	212/240 (88%)	211 (100%)	1 (0%)	0	100	100
2	H	209/240 (87%)	208 (100%)	1 (0%)	0	100	100
2	J	212/240 (88%)	211 (100%)	1 (0%)	0	100	100
2	L	212/240 (88%)	211 (100%)	1 (0%)	0	100	100
2	N	209/240 (87%)	209 (100%)	0	0	100	100
2	P	212/240 (88%)	211 (100%)	1 (0%)	0	100	100
2	R	219/240 (91%)	217 (99%)	2 (1%)	0	100	100
2	T	212/240 (88%)	211 (100%)	1 (0%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	V	217/240 (90%)	214 (99%)	3 (1%)	0	100	100
2	X	212/240 (88%)	210 (99%)	2 (1%)	0	100	100
2	Z	211/240 (88%)	210 (100%)	1 (0%)	0	100	100
All	All	5931/6832 (87%)	5853 (99%)	78 (1%)	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	1	164/192 (85%)	156 (95%)	8 (5%)	25	33
1	A	165/192 (86%)	161 (98%)	4 (2%)	49	61
1	B	164/192 (85%)	158 (96%)	6 (4%)	34	45
1	D	163/192 (85%)	154 (94%)	9 (6%)	21	28
1	F	166/192 (86%)	162 (98%)	4 (2%)	49	61
1	I	164/192 (85%)	160 (98%)	4 (2%)	49	61
1	K	166/192 (86%)	155 (93%)	11 (7%)	16	20
1	M	165/192 (86%)	160 (97%)	5 (3%)	41	53
1	O	164/192 (85%)	160 (98%)	4 (2%)	49	61
1	Q	167/192 (87%)	161 (96%)	6 (4%)	35	46
1	S	164/192 (85%)	158 (96%)	6 (4%)	34	45
1	U	164/192 (85%)	159 (97%)	5 (3%)	41	53
1	W	166/192 (86%)	163 (98%)	3 (2%)	59	71
1	Y	163/192 (85%)	159 (98%)	4 (2%)	47	60
2	2	160/177 (90%)	159 (99%)	1 (1%)	86	91
2	C	160/177 (90%)	157 (98%)	3 (2%)	57	69
2	E	161/177 (91%)	155 (96%)	6 (4%)	34	45
2	G	161/177 (91%)	158 (98%)	3 (2%)	57	69

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	H	160/177 (90%)	156 (98%)	4 (2%)	47	60
2	J	161/177 (91%)	158 (98%)	3 (2%)	57	69
2	L	161/177 (91%)	154 (96%)	7 (4%)	29	38
2	N	159/177 (90%)	155 (98%)	4 (2%)	47	60
2	P	161/177 (91%)	158 (98%)	3 (2%)	57	69
2	R	165/177 (93%)	162 (98%)	3 (2%)	59	71
2	T	161/177 (91%)	156 (97%)	5 (3%)	40	52
2	V	163/177 (92%)	158 (97%)	5 (3%)	40	52
2	X	161/177 (91%)	157 (98%)	4 (2%)	47	60
2	Z	160/177 (90%)	157 (98%)	3 (2%)	57	69
All	All	4559/5166 (88%)	4426 (97%)	133 (3%)	42	54

5 of 133 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	L	444	LEU
1	O	69	ASN
2	Z	430	ASN
2	L	459	ASP
1	M	161	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 48 such sidechains are listed below:

Mol	Chain	Res	Type
1	M	69	ASN
1	O	114	GLN
1	1	114	GLN
1	M	114	GLN
2	N	415	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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	L	301	2	7,9,10	4.83	4 (57%)	9,12,14	5.50	6 (66%)
2	OZT	Z	301	2	7,9,10	4.67	4 (57%)	9,12,14	5.33	6 (66%)
2	OZT	X	301	2	7,9,10	5.00	5 (71%)	9,12,14	5.40	7 (77%)
2	OZT	R	301	2	7,9,10	5.08	5 (71%)	9,12,14	5.09	6 (66%)
2	OZT	C	301	2	7,9,10	4.75	4 (57%)	9,12,14	5.47	6 (66%)
2	OZT	V	301	2	7,9,10	4.53	4 (57%)	9,12,14	5.67	7 (77%)
2	OZT	E	301	2	7,9,10	4.36	4 (57%)	9,12,14	5.19	7 (77%)
2	OZT	P	301	2	7,9,10	4.04	4 (57%)	9,12,14	5.29	6 (66%)
2	OZT	2	301	2	7,9,10	4.88	6 (85%)	9,12,14	5.23	6 (66%)
2	OZT	J	301	2	7,9,10	4.86	4 (57%)	9,12,14	5.42	6 (66%)
2	OZT	T	301	2	7,9,10	4.46	4 (57%)	9,12,14	5.55	6 (66%)
2	OZT	N	301	2	7,9,10	4.46	3 (42%)	9,12,14	5.21	6 (66%)
2	OZT	H	301	2	7,9,10	4.60	4 (57%)	9,12,14	5.55	6 (66%)
2	OZT	G	301	2	7,9,10	4.21	4 (57%)	9,12,14	5.37	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	L	301	2	-	0/1/14/16	0/1/1/1
2	OZT	Z	301	2	-	1/1/14/16	0/1/1/1
2	OZT	X	301	2	-	0/1/14/16	0/1/1/1
2	OZT	R	301	2	-	1/1/14/16	0/1/1/1
2	OZT	C	301	2	-	1/1/14/16	0/1/1/1
2	OZT	V	301	2	-	0/1/14/16	0/1/1/1
2	OZT	E	301	2	-	1/1/14/16	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	OZT	P	301	2	-	1/1/14/16	0/1/1/1
2	OZT	2	301	2	-	1/1/14/16	0/1/1/1
2	OZT	J	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	N	301	2	-	1/1/14/16	0/1/1/1
2	OZT	H	301	2	-	1/1/14/16	0/1/1/1
2	OZT	G	301	2	-	1/1/14/16	0/1/1/1

The worst 5 of 59 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	301	OZT	O1-C5	10.85	1.51	1.36
2	X	301	OZT	O1-C5	10.58	1.50	1.36
2	L	301	OZT	O1-C5	10.33	1.50	1.36
2	T	301	OZT	O1-C5	9.91	1.49	1.36
2	R	301	OZT	O1-C5	9.54	1.49	1.36

The worst 5 of 88 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	301	OZT	O1-C5-N	9.10	117.50	109.86
2	T	301	OZT	O1-C5-N	9.00	117.41	109.86
2	N	301	OZT	O1-C5-N	8.95	117.37	109.86
2	P	301	OZT	O1-C5-N	8.88	117.31	109.86
2	V	301	OZT	O1-C2-CA	8.78	112.05	103.58

There are no chirality outliers.

5 of 11 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	Z	301	OZT	O-C-CA-C2
2	R	301	OZT	O-C-CA-C2
2	C	301	OZT	O-C-CA-C2
2	E	301	OZT	O-C-CA-C2
2	P	301	OZT	O-C-CA-C2

There are no ring outliers.

11 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	L	301	OZT	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	Z	301	OZT	1	0
2	X	301	OZT	1	0
2	R	301	OZT	3	0
2	C	301	OZT	2	0
2	V	301	OZT	2	0
2	P	301	OZT	4	0
2	2	301	OZT	3	0
2	T	301	OZT	1	0
2	N	301	OZT	3	0
2	H	301	OZT	2	0

## 5.5 Carbohydrates

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

102 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	H	53	-	4,4,4	0.32	0	4,4,4	0.36	0
3	DMF	E	44	-	4,4,4	0.28	0	4,4,4	0.52	0
3	DMF	2	78	-	4,4,4	0.20	0	4,4,4	0.39	0
3	DMF	P	100	-	4,4,4	0.48	0	4,4,4	0.32	0
3	DMF	S	251	-	4,4,4	0.30	0	4,4,4	0.40	0
3	DMF	U	249	-	4,4,4	0.51	0	4,4,4	0.22	0
3	DMF	B	250	-	4,4,4	0.84	0	4,4,4	0.28	0
3	DMF	N	24	-	4,4,4	0.45	0	4,4,4	0.32	0
3	DMF	P	61	-	4,4,4	0.73	0	4,4,4	0.29	0
3	DMF	E	70	-	4,4,4	0.32	0	4,4,4	0.51	0
3	DMF	O	249	-	4,4,4	0.26	0	4,4,4	0.64	0
3	DMF	B	249	-	4,4,4	0.19	0	4,4,4	0.40	0
3	DMF	C	17	-	4,4,4	0.26	0	4,4,4	0.40	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	DMF	K	250	-	4,4,4	0.56	0	4,4,4	0.35	0
3	DMF	H	52	-	4,4,4	0.35	0	4,4,4	0.52	0
3	DMF	E	55	-	4,4,4	0.43	0	4,4,4	0.33	0
3	DMF	R	89	-	4,4,4	0.29	0	4,4,4	0.55	0
3	DMF	M	250	-	4,4,4	0.70	0	4,4,4	0.51	0
3	DMF	T	62	-	4,4,4	0.46	0	4,4,4	0.30	0
3	DMF	P	23	-	4,4,4	0.21	0	4,4,4	0.35	0
3	DMF	D	250	-	4,4,4	0.65	0	4,4,4	0.32	0
3	DMF	K	249	-	4,4,4	0.70	0	4,4,4	0.27	0
3	DMF	H	102	-	4,4,4	0.46	0	4,4,4	0.38	0
3	DMF	N	2	-	4,4,4	0.17	0	4,4,4	0.41	0
3	DMF	E	83	-	4,4,4	0.28	0	4,4,4	0.72	0
3	DMF	H	19	-	4,4,4	0.47	0	4,4,4	0.29	0
3	DMF	C	43	-	4,4,4	0.91	0	4,4,4	0.34	0
3	DMF	H	31	-	4,4,4	0.83	0	4,4,4	0.31	0
3	DMF	P	74	-	4,4,4	0.38	0	4,4,4	0.18	0
3	DMF	G	39	-	4,4,4	0.70	0	4,4,4	0.33	0
3	DMF	F	249	-	4,4,4	0.52	0	4,4,4	0.43	0
3	DMF	D	251	-	4,4,4	0.44	0	4,4,4	0.47	0
3	DMF	2	66	-	4,4,4	0.70	0	4,4,4	0.26	0
3	DMF	R	3	-	4,4,4	0.26	0	4,4,4	0.43	0
3	DMF	W	249	-	4,4,4	0.33	0	4,4,4	0.37	0
3	DMF	N	36	-	4,4,4	0.32	0	4,4,4	0.44	0
3	DMF	C	73	-	4,4,4	0.26	0	4,4,4	0.34	0
3	DMF	S	250	-	4,4,4	0.28	0	4,4,4	0.41	0
3	DMF	G	96	-	4,4,4	0.77	0	4,4,4	0.31	0
3	DMF	U	250	-	4,4,4	0.29	0	4,4,4	0.47	0
3	DMF	D	249	-	4,4,4	0.28	0	4,4,4	0.32	0
3	DMF	1	251	-	4,4,4	0.45	0	4,4,4	0.61	0
3	DMF	V	86	-	4,4,4	0.27	0	4,4,4	0.47	0
3	DMF	Q	250	-	4,4,4	0.29	0	4,4,4	0.52	0
3	DMF	I	250	-	4,4,4	0.45	0	4,4,4	0.26	0
3	DMF	C	64	-	4,4,4	0.26	0	4,4,4	0.44	0
3	DMF	L	60	-	4,4,4	0.45	0	4,4,4	0.30	0
3	DMF	V	16	-	4,4,4	0.35	0	4,4,4	0.55	0
3	DMF	V	65	-	4,4,4	0.86	0	4,4,4	0.28	0
3	DMF	N	37	-	4,4,4	0.66	0	4,4,4	0.39	0
3	DMF	R	54	-	4,4,4	0.37	0	4,4,4	0.41	0
3	DMF	J	82	-	4,4,4	0.51	0	4,4,4	0.33	0
3	DMF	C	48	-	4,4,4	0.47	0	4,4,4	0.28	0
3	DMF	G	20	-	4,4,4	0.49	0	4,4,4	0.34	0
3	DMF	S	249	-	4,4,4	0.57	0	4,4,4	0.20	0
3	DMF	F	250	-	4,4,4	0.33	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	X	88	-	4,4,4	0.46	0	4,4,4	0.45	0
3	DMF	C	5	-	4,4,4	0.31	0	4,4,4	0.55	0
3	DMF	J	6	-	4,4,4	0.26	0	4,4,4	0.41	0
3	DMF	M	249	-	4,4,4	0.56	0	4,4,4	0.39	0
3	DMF	I	249	-	4,4,4	0.72	0	4,4,4	0.37	0
3	DMF	X	67	-	4,4,4	0.70	0	4,4,4	0.30	0
3	DMF	N	97	-	4,4,4	0.87	0	4,4,4	0.44	0
3	DMF	O	250	-	4,4,4	0.29	0	4,4,4	0.44	0
3	DMF	T	92	-	4,4,4	0.82	0	4,4,4	0.35	0
3	DMF	Z	79	-	4,4,4	0.85	0	4,4,4	0.45	0
3	DMF	U	252	-	4,4,4	0.82	0	4,4,4	0.36	0
3	DMF	E	95	-	4,4,4	1.07	0	4,4,4	0.41	0
3	DMF	H	14	-	4,4,4	0.56	0	4,4,4	0.31	0
3	DMF	R	68	-	4,4,4	0.25	0	4,4,4	0.50	0
3	DMF	T	94	-	4,4,4	0.51	0	4,4,4	0.35	0
3	DMF	Z	91	-	4,4,4	0.30	0	4,4,4	0.56	0
3	DMF	C	28	-	4,4,4	0.53	0	4,4,4	0.29	0
3	DMF	N	99	-	4,4,4	0.89	0	4,4,4	0.45	0
3	DMF	T	35	-	4,4,4	0.33	0	4,4,4	0.37	0
3	DMF	E	32	-	4,4,4	0.68	0	4,4,4	0.33	0
3	DMF	Q	249	-	4,4,4	0.43	0	4,4,4	0.34	0
3	DMF	J	59	-	4,4,4	0.22	0	4,4,4	0.37	0
3	DMF	N	21	-	4,4,4	0.24	0	4,4,4	0.41	0
3	DMF	B	251	-	4,4,4	0.66	0	4,4,4	0.22	0
3	DMF	A	249	-	4,4,4	0.55	0	4,4,4	0.34	0
3	DMF	H	41	-	4,4,4	0.53	0	4,4,4	0.35	0
3	DMF	2	58	-	4,4,4	0.77	0	4,4,4	0.30	0
3	DMF	T	46	-	4,4,4	0.51	0	4,4,4	0.35	0
3	DMF	L	4	-	4,4,4	0.42	0	4,4,4	0.29	0
3	DMF	1	250	-	4,4,4	0.35	0	4,4,4	0.27	0
3	DMF	C	15	-	4,4,4	0.38	0	4,4,4	0.41	0
3	DMF	W	250	-	4,4,4	0.69	0	4,4,4	0.31	0
3	DMF	Z	27	-	4,4,4	0.15	0	4,4,4	0.37	0
3	DMF	X	25	-	4,4,4	0.57	0	4,4,4	0.44	0
3	DMF	1	249	-	4,4,4	0.51	0	4,4,4	0.39	0
3	DMF	D	252	-	4,4,4	0.24	0	4,4,4	0.35	0
3	DMF	U	251	-	4,4,4	0.85	0	4,4,4	0.27	0
3	DMF	G	1	-	4,4,4	0.35	0	4,4,4	0.57	0
3	DMF	Z	50	-	4,4,4	0.23	0	4,4,4	0.40	0
3	DMF	Z	71	-	4,4,4	0.47	0	4,4,4	0.33	0
3	DMF	V	90	-	4,4,4	0.25	0	4,4,4	0.34	0
3	DMF	A	250	-	4,4,4	0.62	0	4,4,4	0.44	0
3	DMF	Y	249	-	4,4,4	0.63	0	4,4,4	0.44	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	DMF	Z	69	-	4,4,4	0.56	0	4,4,4	0.30	0
3	DMF	P	85	-	4,4,4	0.80	0	4,4,4	0.37	0
3	DMF	L	9	-	4,4,4	0.20	0	4,4,4	0.44	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	H	53	-	-	2/2/2/2	-
3	DMF	E	44	-	-	2/2/2/2	-
3	DMF	2	78	-	-	0/2/2/2	-
3	DMF	P	100	-	-	0/2/2/2	-
3	DMF	S	251	-	-	2/2/2/2	-
3	DMF	U	249	-	-	0/2/2/2	-
3	DMF	B	250	-	-	0/2/2/2	-
3	DMF	N	24	-	-	0/2/2/2	-
3	DMF	P	61	-	-	0/2/2/2	-
3	DMF	E	70	-	-	2/2/2/2	-
3	DMF	O	249	-	-	2/2/2/2	-
3	DMF	B	249	-	-	2/2/2/2	-
3	DMF	C	17	-	-	0/2/2/2	-
3	DMF	K	250	-	-	0/2/2/2	-
3	DMF	H	52	-	-	2/2/2/2	-
3	DMF	E	55	-	-	0/2/2/2	-
3	DMF	R	89	-	-	2/2/2/2	-
3	DMF	M	250	-	-	0/2/2/2	-
3	DMF	T	62	-	-	0/2/2/2	-
3	DMF	P	23	-	-	0/2/2/2	-
3	DMF	D	250	-	-	0/2/2/2	-
3	DMF	K	249	-	-	0/2/2/2	-
3	DMF	H	102	-	-	0/2/2/2	-
3	DMF	N	2	-	-	2/2/2/2	-
3	DMF	E	83	-	-	2/2/2/2	-
3	DMF	H	19	-	-	0/2/2/2	-
3	DMF	C	43	-	-	0/2/2/2	-
3	DMF	H	31	-	-	0/2/2/2	-
3	DMF	P	74	-	-	0/2/2/2	-
3	DMF	G	39	-	-	0/2/2/2	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	DMF	F	249	-	-	0/2/2/2	-
3	DMF	D	251	-	-	0/2/2/2	-
3	DMF	2	66	-	-	0/2/2/2	-
3	DMF	R	3	-	-	2/2/2/2	-
3	DMF	W	249	-	-	2/2/2/2	-
3	DMF	N	36	-	-	0/2/2/2	-
3	DMF	C	73	-	-	2/2/2/2	-
3	DMF	S	250	-	-	2/2/2/2	-
3	DMF	G	96	-	-	0/2/2/2	-
3	DMF	U	250	-	-	2/2/2/2	-
3	DMF	D	249	-	-	2/2/2/2	-
3	DMF	1	251	-	-	0/2/2/2	-
3	DMF	V	86	-	-	0/2/2/2	-
3	DMF	Q	250	-	-	2/2/2/2	-
3	DMF	I	250	-	-	0/2/2/2	-
3	DMF	C	64	-	-	2/2/2/2	-
3	DMF	L	60	-	-	0/2/2/2	-
3	DMF	V	16	-	-	2/2/2/2	-
3	DMF	V	65	-	-	0/2/2/2	-
3	DMF	N	37	-	-	0/2/2/2	-
3	DMF	R	54	-	-	0/2/2/2	-
3	DMF	J	82	-	-	0/2/2/2	-
3	DMF	C	48	-	-	0/2/2/2	-
3	DMF	G	20	-	-	0/2/2/2	-
3	DMF	S	249	-	-	0/2/2/2	-
3	DMF	F	250	-	-	2/2/2/2	-
3	DMF	X	88	-	-	0/2/2/2	-
3	DMF	C	5	-	-	2/2/2/2	-
3	DMF	J	6	-	-	2/2/2/2	-
3	DMF	M	249	-	-	0/2/2/2	-
3	DMF	I	249	-	-	0/2/2/2	-
3	DMF	X	67	-	-	0/2/2/2	-
3	DMF	N	97	-	-	0/2/2/2	-
3	DMF	O	250	-	-	2/2/2/2	-
3	DMF	T	92	-	-	0/2/2/2	-
3	DMF	Z	79	-	-	0/2/2/2	-
3	DMF	U	252	-	-	0/2/2/2	-
3	DMF	E	95	-	-	0/2/2/2	-
3	DMF	H	14	-	-	0/2/2/2	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	DMF	R	68	-	-	2/2/2/2	-
3	DMF	T	94	-	-	0/2/2/2	-
3	DMF	Z	91	-	-	2/2/2/2	-
3	DMF	C	28	-	-	0/2/2/2	-
3	DMF	N	99	-	-	0/2/2/2	-
3	DMF	T	35	-	-	2/2/2/2	-
3	DMF	E	32	-	-	0/2/2/2	-
3	DMF	Q	249	-	-	0/2/2/2	-
3	DMF	J	59	-	-	2/2/2/2	-
3	DMF	N	21	-	-	2/2/2/2	-
3	DMF	B	251	-	-	0/2/2/2	-
3	DMF	A	249	-	-	0/2/2/2	-
3	DMF	H	41	-	-	0/2/2/2	-
3	DMF	2	58	-	-	0/2/2/2	-
3	DMF	T	46	-	-	0/2/2/2	-
3	DMF	L	4	-	-	0/2/2/2	-
3	DMF	1	250	-	-	0/2/2/2	-
3	DMF	C	15	-	-	0/2/2/2	-
3	DMF	W	250	-	-	0/2/2/2	-
3	DMF	Z	27	-	-	2/2/2/2	-
3	DMF	X	25	-	-	0/2/2/2	-
3	DMF	1	249	-	-	0/2/2/2	-
3	DMF	D	252	-	-	2/2/2/2	-
3	DMF	U	251	-	-	0/2/2/2	-
3	DMF	G	1	-	-	2/2/2/2	-
3	DMF	Z	50	-	-	0/2/2/2	-
3	DMF	Z	71	-	-	0/2/2/2	-
3	DMF	V	90	-	-	2/2/2/2	-
3	DMF	A	250	-	-	0/2/2/2	-
3	DMF	Y	249	-	-	0/2/2/2	-
3	DMF	Z	69	-	-	0/2/2/2	-
3	DMF	P	85	-	-	0/2/2/2	-
3	DMF	L	9	-	-	2/2/2/2	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 66 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	N	2	DMF	O-C-N-C1
3	D	252	DMF	O-C-N-C1
3	D	252	DMF	O-C-N-C2
3	R	89	DMF	O-C-N-C1
3	C	73	DMF	O-C-N-C2

There are no ring outliers.

57 monomers are involved in 107 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	H	53	DMF	2	0
3	2	78	DMF	1	0
3	B	250	DMF	1	0
3	P	61	DMF	1	0
3	E	70	DMF	2	0
3	O	249	DMF	2	0
3	B	249	DMF	1	0
3	C	17	DMF	1	0
3	K	250	DMF	2	0
3	E	55	DMF	1	0
3	R	89	DMF	1	0
3	P	23	DMF	1	0
3	N	2	DMF	2	0
3	H	19	DMF	4	0
3	C	43	DMF	1	0
3	H	31	DMF	1	0
3	G	39	DMF	1	0
3	D	251	DMF	1	0
3	W	249	DMF	1	0
3	N	36	DMF	2	0
3	C	73	DMF	7	0
3	S	250	DMF	1	0
3	G	96	DMF	3	0
3	U	250	DMF	1	0
3	1	251	DMF	2	0
3	C	64	DMF	6	0
3	L	60	DMF	1	0
3	V	16	DMF	1	0
3	J	82	DMF	1	0
3	G	20	DMF	3	0
3	F	250	DMF	1	0
3	C	5	DMF	5	0
3	J	6	DMF	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	M	249	DMF	1	0
3	X	67	DMF	1	0
3	N	97	DMF	3	0
3	O	250	DMF	4	0
3	T	92	DMF	1	0
3	Z	79	DMF	1	0
3	U	252	DMF	1	0
3	E	95	DMF	1	0
3	R	68	DMF	1	0
3	T	94	DMF	3	0
3	Z	91	DMF	3	0
3	T	35	DMF	5	0
3	E	32	DMF	1	0
3	H	41	DMF	1	0
3	L	4	DMF	1	0
3	1	250	DMF	1	0
3	Z	27	DMF	2	0
3	D	252	DMF	1	0
3	U	251	DMF	2	0
3	G	1	DMF	1	0
3	Z	71	DMF	1	0
3	A	250	DMF	2	0
3	Z	69	DMF	3	0
3	L	9	DMF	3	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.



## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	1	215/248 (86%)	0.41	19 (8%) 10 7	20, 55, 92, 101	0
1	A	216/248 (87%)	0.66	35 (16%) 1 1	21, 56, 100, 109	0
1	B	214/248 (86%)	0.43	16 (7%) 14 11	22, 56, 98, 108	0
1	D	213/248 (85%)	0.65	27 (12%) 3 2	21, 56, 96, 105	0
1	F	217/248 (87%)	0.44	14 (6%) 18 15	22, 55, 91, 102	0
1	I	215/248 (86%)	0.46	19 (8%) 10 7	23, 56, 98, 107	0
1	K	217/248 (87%)	0.53	24 (11%) 5 3	19, 57, 94, 109	0
1	M	216/248 (87%)	0.40	13 (6%) 21 18	21, 55, 92, 99	0
1	O	215/248 (86%)	0.49	20 (9%) 8 6	21, 56, 92, 102	0
1	Q	218/248 (87%)	0.39	16 (7%) 15 11	21, 55, 90, 101	0
1	S	215/248 (86%)	0.61	32 (14%) 2 1	21, 57, 102, 112	0
1	U	215/248 (86%)	0.45	13 (6%) 21 18	22, 55, 96, 106	0
1	W	217/248 (87%)	0.49	21 (9%) 7 5	22, 56, 93, 99	0
1	Y	213/248 (85%)	0.74	30 (14%) 2 1	23, 57, 99, 111	0
2	2	214/240 (89%)	-0.51	4 (1%) 66 63	10, 20, 43, 73	0
2	C	214/240 (89%)	-0.38	5 (2%) 60 56	8, 20, 46, 76	0
2	E	215/240 (89%)	-0.51	3 (1%) 75 73	10, 20, 45, 76	0
2	G	215/240 (89%)	-0.58	1 (0%) 91 91	10, 21, 47, 75	0
2	H	212/240 (88%)	-0.49	2 (0%) 84 83	11, 22, 45, 70	0
2	J	215/240 (89%)	-0.37	3 (1%) 75 73	10, 21, 46, 70	0
2	L	215/240 (89%)	-0.45	2 (0%) 84 83	10, 21, 45, 72	0
2	N	212/240 (88%)	-0.50	1 (0%) 91 91	9, 21, 43, 67	0
2	P	215/240 (89%)	-0.42	6 (2%) 53 49	10, 23, 47, 73	0
2	R	222/240 (92%)	-0.50	2 (0%) 84 83	8, 19, 44, 73	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
2	T	215/240 (89%)	-0.35	4 (1%) 66 63	9, 22, 47, 80	0
2	V	220/240 (91%)	-0.57	5 (2%) 60 56	8, 20, 44, 74	0
2	X	215/240 (89%)	-0.48	4 (1%) 66 63	10, 22, 46, 79	0
2	Z	214/240 (89%)	-0.43	2 (0%) 84 83	10, 23, 46, 68	0
All	All	6029/6832 (88%)	0.02	343 (5%) 23 20	8, 34, 89, 112	0

The worst 5 of 343 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	Y	12	ALA	9.2
1	S	188	LEU	7.4
1	F	202	THR	7.2
1	B	205	VAL	7.0
1	U	204	GLY	6.5

## 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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	OZT	R	301	9/10	0.87	0.19	23,29,35,38	0
2	OZT	V	301	9/10	0.90	0.15	23,30,35,36	0
2	OZT	C	301	9/10	0.91	0.15	19,28,34,37	0
2	OZT	2	301	9/10	0.91	0.16	23,30,34,35	0
2	OZT	L	301	9/10	0.92	0.13	25,29,34,35	0
2	OZT	P	301	9/10	0.92	0.15	25,29,34,39	0
2	OZT	X	301	9/10	0.92	0.14	28,31,35,36	0
2	OZT	J	301	9/10	0.92	0.16	24,30,34,38	0
2	OZT	N	301	9/10	0.92	0.13	23,28,35,38	0
2	OZT	E	301	9/10	0.94	0.13	25,31,33,36	0
2	OZT	H	301	9/10	0.94	0.12	24,30,33,33	0
2	OZT	Z	301	9/10	0.95	0.12	25,28,32,33	0
2	OZT	T	301	9/10	0.96	0.11	26,29,32,34	0
2	OZT	G	301	9/10	0.96	0.11	24,30,34,37	0

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	DMF	D	249	5/5	0.56	0.45	83,83,84,84	0
3	DMF	T	35	5/5	0.59	0.36	75,75,76,77	0
3	DMF	D	252	5/5	0.60	0.33	50,50,54,55	0
3	DMF	H	31	5/5	0.61	0.55	64,66,68,68	0
3	DMF	T	94	5/5	0.68	0.44	104,104,104,104	0
3	DMF	G	39	5/5	0.69	0.32	55,57,59,60	0
3	DMF	W	250	5/5	0.70	0.35	61,62,64,64	0
3	DMF	F	250	5/5	0.70	0.28	68,69,71,71	0
3	DMF	E	32	5/5	0.72	0.43	60,62,63,65	0
3	DMF	Q	250	5/5	0.73	0.32	69,70,70,71	0
3	DMF	B	251	5/5	0.74	0.27	61,64,64,64	0
3	DMF	2	58	5/5	0.74	0.38	60,62,64,64	0
3	DMF	S	250	5/5	0.75	0.28	48,49,51,51	0
3	DMF	G	20	5/5	0.75	0.35	46,50,51,53	0
3	DMF	S	249	5/5	0.76	0.33	63,64,65,66	0
3	DMF	C	48	5/5	0.76	0.31	68,69,70,70	0
3	DMF	C	43	5/5	0.77	0.25	57,57,59,59	0
3	DMF	R	54	5/5	0.78	0.32	46,48,49,51	0
3	DMF	N	99	5/5	0.78	0.25	50,52,53,54	0
3	DMF	J	82	5/5	0.79	0.30	50,52,54,57	0
3	DMF	2	66	5/5	0.79	0.33	69,70,70,71	0
3	DMF	N	36	5/5	0.80	0.31	50,53,54,57	0
3	DMF	V	65	5/5	0.80	0.28	60,60,61,61	0
3	DMF	G	96	5/5	0.80	0.29	79,80,80,81	0
3	DMF	D	251	5/5	0.81	0.27	51,53,54,56	0
3	DMF	O	250	5/5	0.81	0.32	59,60,60,61	0
3	DMF	A	250	5/5	0.81	0.25	52,54,56,59	0
3	DMF	E	95	5/5	0.82	0.26	46,49,51,55	0
3	DMF	B	250	5/5	0.82	0.19	39,39,43,45	0
3	DMF	X	67	5/5	0.83	0.25	58,59,60,60	0
3	DMF	N	97	5/5	0.83	0.27	31,36,38,38	0
3	DMF	P	61	5/5	0.83	0.28	58,59,61,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	DMF	K	250	5/5	0.83	0.29	59,61,62,63	0
3	DMF	R	3	5/5	0.83	0.33	63,63,65,65	0
3	DMF	1	250	5/5	0.83	0.20	60,60,61,61	0
3	DMF	1	251	5/5	0.83	0.26	45,48,49,49	0
3	DMF	H	41	5/5	0.84	0.28	62,63,63,64	0
3	DMF	Z	27	5/5	0.84	0.34	57,62,64,65	0
3	DMF	H	19	5/5	0.84	0.27	52,53,55,58	0
3	DMF	T	62	5/5	0.84	0.30	56,58,58,60	0
3	DMF	Y	249	5/5	0.85	0.20	58,59,61,62	0
3	DMF	X	25	5/5	0.86	0.24	47,49,50,51	0
3	DMF	C	5	5/5	0.86	0.32	77,77,78,78	0
3	DMF	P	100	5/5	0.86	0.23	53,54,54,55	0
3	DMF	W	249	5/5	0.86	0.26	77,77,78,78	0
3	DMF	H	52	5/5	0.87	0.26	65,66,66,67	0
3	DMF	S	251	5/5	0.87	0.20	69,70,70,70	0
3	DMF	U	251	5/5	0.87	0.22	45,45,46,48	0
3	DMF	N	37	5/5	0.87	0.29	63,64,65,67	0
3	DMF	C	73	5/5	0.87	0.24	53,54,54,55	0
3	DMF	X	88	5/5	0.88	0.24	46,48,50,51	0
3	DMF	C	15	5/5	0.88	0.29	51,53,54,56	0
3	DMF	R	89	5/5	0.88	0.26	52,53,53,54	0
3	DMF	L	9	5/5	0.88	0.28	61,63,64,65	0
3	DMF	U	252	5/5	0.89	0.18	60,60,61,61	0
3	DMF	2	78	5/5	0.89	0.19	43,44,46,48	0
3	DMF	L	60	5/5	0.89	0.22	57,57,58,59	0
3	DMF	U	250	5/5	0.89	0.14	71,71,72,72	0
3	DMF	F	249	5/5	0.89	0.27	55,55,56,56	0
3	DMF	O	249	5/5	0.89	0.22	42,46,47,49	0
3	DMF	C	64	5/5	0.90	0.26	60,60,60,61	0
3	DMF	N	21	5/5	0.90	0.26	75,76,76,76	0
3	DMF	E	70	5/5	0.90	0.26	77,77,78,78	0
3	DMF	R	68	5/5	0.90	0.23	53,56,57,57	0
3	DMF	P	74	5/5	0.90	0.29	72,73,74,74	0
3	DMF	H	102	5/5	0.90	0.26	73,73,74,74	0
3	DMF	Z	69	5/5	0.90	0.28	69,70,71,71	0
3	DMF	E	83	5/5	0.90	0.24	64,65,65,66	0
3	DMF	P	23	5/5	0.91	0.30	60,60,61,63	0
3	DMF	D	250	5/5	0.91	0.24	67,67,67,68	0
3	DMF	Z	91	5/5	0.91	0.24	54,55,55,56	0
3	DMF	Z	50	5/5	0.91	0.21	48,49,50,52	0
3	DMF	Z	71	5/5	0.91	0.26	52,52,54,56	0
3	DMF	C	28	5/5	0.91	0.21	53,54,56,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	DMF	T	92	5/5	0.91	0.29	41,44,45,46	0
3	DMF	B	249	5/5	0.91	0.22	49,52,53,55	0
3	DMF	P	85	5/5	0.91	0.23	52,53,54,54	0
3	DMF	C	17	5/5	0.91	0.17	37,38,41,42	0
3	DMF	N	2	5/5	0.92	0.23	44,45,48,50	0
3	DMF	H	14	5/5	0.92	0.24	63,63,64,64	0
3	DMF	V	90	5/5	0.92	0.20	66,66,68,71	0
3	DMF	V	16	5/5	0.92	0.23	48,50,51,52	0
3	DMF	I	250	5/5	0.92	0.16	48,51,51,52	0
3	DMF	M	250	5/5	0.92	0.19	35,37,37,38	0
3	DMF	1	249	5/5	0.92	0.19	56,57,58,59	0
3	DMF	I	249	5/5	0.92	0.19	42,43,44,45	0
3	DMF	Z	79	5/5	0.93	0.19	38,38,39,40	0
3	DMF	G	1	5/5	0.93	0.24	38,42,43,46	0
3	DMF	J	6	5/5	0.93	0.22	53,54,55,57	0
3	DMF	E	44	5/5	0.93	0.19	42,44,46,46	0
3	DMF	N	24	5/5	0.93	0.15	41,42,44,46	0
3	DMF	Q	249	5/5	0.93	0.21	52,52,53,54	0
3	DMF	K	249	5/5	0.93	0.17	37,40,41,41	0
3	DMF	H	53	5/5	0.93	0.21	63,64,65,65	0
3	DMF	V	86	5/5	0.93	0.23	44,44,45,48	0
3	DMF	A	249	5/5	0.94	0.15	54,55,55,56	0
3	DMF	T	46	5/5	0.94	0.18	45,46,47,48	0
3	DMF	U	249	5/5	0.94	0.23	46,47,48,49	0
3	DMF	M	249	5/5	0.95	0.17	43,43,44,46	0
3	DMF	L	4	5/5	0.95	0.13	47,47,47,48	0
3	DMF	J	59	5/5	0.96	0.15	65,65,66,66	0
3	DMF	E	55	5/5	0.96	0.16	41,41,42,42	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.