



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 30, 2020 – 02:07 PM BST

PDB ID : 3HF9
Title : Crystal Structure of Mycobacterium Tuberculosis Proteasome open-gate mutant modified by inhibitor GL1
Authors : Li, D.; Li, H.
Deposited on : 2009-05-11
Resolution : 2.88 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The 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 : **FAILED**
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13

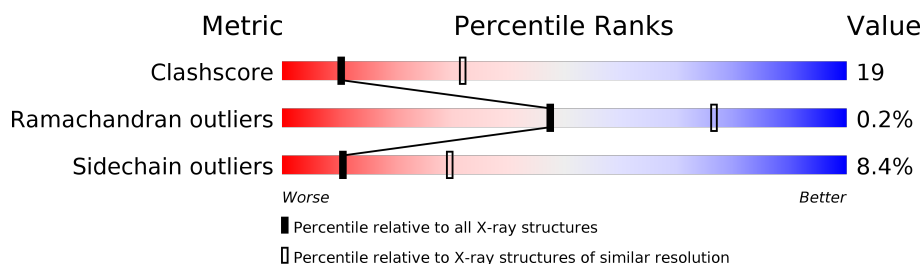
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.88 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))
Clashscore	141614	2947 (2.90-2.86)
Ramachandran outliers	138981	2868 (2.90-2.86)
Sidechain outliers	138945	2871 (2.90-2.86)















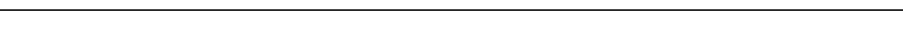




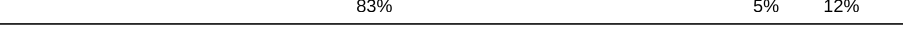





The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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 $\leq 5\%$.

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	1	240	57% 30% • 12%
1	3	240	61% 24% • 13%
1	A	240	50% 34% • 12%
1	B	240	50% 33% 5% 12%
1	D	240	43% 41% • 13%
1	F	240	48% 27% 6% 20%
1	I	240	60% 25% • 12%
1	K	240	55% 30% • 12%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	M	240	
1	O	240	
1	Q	240	
1	S	240	
1	U	240	
1	W	240	
1	Y	240	
1	a	240	
1	b	240	
1	d	240	
1	f	240	
1	i	240	
1	k	240	
1	m	240	
1	o	240	
1	q	240	
1	s	240	
1	u	240	
1	w	240	
1	y	240	
2	2	240	
2	4	240	
2	C	240	
2	E	240	
2	G	240	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
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	
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	2	1	-	-	X	-
2	OZT	4	301	-	-	X	-
2	OZT	E	1	-	-	X	-
2	OZT	H	1	-	-	X	-
2	OZT	L	1	-	-	X	-
2	OZT	X	1	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 90443 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	211	Total	C	N	O	S	0	0	0
			1633	1023	299	308	3			
1	B	211	Total	C	N	O	S	0	0	0
			1633	1023	299	308	3			
1	D	210	Total	C	N	O	S	0	0	0
			1625	1017	298	307	3			
1	F	193	Total	C	N	O	S	0	0	0
			1490	939	267	282	2			
1	I	212	Total	C	N	O	S	0	0	0
			1640	1028	300	309	3			
1	K	211	Total	C	N	O	S	0	0	0
			1633	1023	299	308	3			
1	M	205	Total	C	N	O	S	0	0	0
			1589	995	292	299	3			
1	O	211	Total	C	N	O	S	0	0	0
			1633	1023	299	308	3			
1	Q	211	Total	C	N	O	S	0	0	0
			1633	1023	299	308	3			
1	S	211	Total	C	N	O	S	0	0	0
			1633	1023	299	308	3			
1	U	211	Total	C	N	O	S	0	0	0
			1633	1023	299	308	3			
1	W	193	Total	C	N	O	S	0	0	0
			1487	936	267	282	2			
1	Y	210	Total	C	N	O	S	0	0	0
			1625	1017	298	307	3			
1	1	211	Total	C	N	O	S	0	0	0
			1633	1023	299	308	3			
1	a	211	Total	C	N	O	S	0	0	0
			1633	1023	299	308	3			
1	b	211	Total	C	N	O	S	0	0	0
			1633	1023	299	308	3			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	d	211	Total 1633	C 1023	N 299	O 308	S 3	0	0	0
1	f	211	Total 1633	C 1023	N 299	O 308	S 3	0	0	0
1	i	211	Total 1633	C 1023	N 299	O 308	S 3	0	0	0
1	k	211	Total 1633	C 1023	N 299	O 308	S 3	0	0	0
1	m	208	Total 1612	C 1008	N 296	O 305	S 3	0	0	0
1	o	211	Total 1633	C 1023	N 299	O 308	S 3	0	0	0
1	q	211	Total 1633	C 1023	N 299	O 308	S 3	0	0	0
1	s	211	Total 1633	C 1023	N 299	O 308	S 3	0	0	0
1	u	211	Total 1633	C 1023	N 299	O 308	S 3	0	0	0
1	w	211	Total 1633	C 1023	N 299	O 308	S 3	0	0	0
1	y	211	Total 1633	C 1023	N 299	O 308	S 3	0	0	0
1	3	210	Total 1625	C 1017	N 298	O 307	S 3	0	0	0

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	9	MET	-	INITIATING METHIONINE	UNP O33244
B	9	MET	-	INITIATING METHIONINE	UNP O33244
D	9	MET	-	INITIATING METHIONINE	UNP O33244
F	9	MET	-	INITIATING METHIONINE	UNP O33244
I	9	MET	-	INITIATING METHIONINE	UNP O33244
K	9	MET	-	INITIATING METHIONINE	UNP O33244
M	9	MET	-	INITIATING METHIONINE	UNP O33244
O	9	MET	-	INITIATING METHIONINE	UNP O33244
Q	9	MET	-	INITIATING METHIONINE	UNP O33244
S	9	MET	-	INITIATING METHIONINE	UNP O33244
U	9	MET	-	INITIATING METHIONINE	UNP O33244
W	9	MET	-	INITIATING METHIONINE	UNP O33244
Y	9	MET	-	INITIATING METHIONINE	UNP O33244
1	9	MET	-	INITIATING METHIONINE	UNP O33244
a	309	MET	-	INITIATING METHIONINE	UNP O33244

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
b	309	MET	-	INITIATING METHIONINE	UNP O33244
d	309	MET	-	INITIATING METHIONINE	UNP O33244
f	309	MET	-	INITIATING METHIONINE	UNP O33244
i	309	MET	-	INITIATING METHIONINE	UNP O33244
k	309	MET	-	INITIATING METHIONINE	UNP O33244
m	309	MET	-	INITIATING METHIONINE	UNP O33244
o	309	MET	-	INITIATING METHIONINE	UNP O33244
q	309	MET	-	INITIATING METHIONINE	UNP O33244
s	309	MET	-	INITIATING METHIONINE	UNP O33244
u	309	MET	-	INITIATING METHIONINE	UNP O33244
w	309	MET	-	INITIATING METHIONINE	UNP O33244
y	309	MET	-	INITIATING METHIONINE	UNP O33244
3	309	MET	-	INITIATING METHIONINE	UNP O33244

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	217	Total	C	N	O	S	0	0	0
			1606	1007	276	319	4			
2	C	217	Total	C	N	O	S	0	0	0
			1606	1007	276	319	4			
2	E	217	Total	C	N	O	S	0	0	0
			1606	1007	276	319	4			
2	G	217	Total	C	N	O	S	0	0	0
			1606	1007	276	319	4			
2	J	217	Total	C	N	O	S	0	0	0
			1606	1007	276	319	4			
2	L	217	Total	C	N	O	S	0	0	0
			1606	1007	276	319	4			
2	N	217	Total	C	N	O	S	0	0	0
			1606	1007	276	319	4			
2	P	217	Total	C	N	O	S	0	0	0
			1606	1007	276	319	4			
2	R	217	Total	C	N	O	S	0	0	0
			1606	1007	276	319	4			
2	T	217	Total	C	N	O	S	0	0	0
			1606	1007	276	319	4			
2	V	218	Total	C	N	O	S	0	0	0
			1610	1009	277	320	4			
2	X	217	Total	C	N	O	S	0	0	0
			1606	1007	276	319	4			
2	Z	217	Total	C	N	O	S	0	0	0
			1606	1007	276	319	4			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	2	217	Total	C	N	O	S	0	0	0
			1606	1007	276	319	4			
2	h	214	Total	C	N	O	S	0	0	0
			1588	995	273	316	4			
2	c	215	Total	C	N	O	S	0	0	0
			1596	1001	274	317	4			
2	e	217	Total	C	N	O	S	0	0	0
			1606	1007	276	319	4			
2	g	217	Total	C	N	O	S	0	0	0
			1606	1007	276	319	4			
2	j	217	Total	C	N	O	S	0	0	0
			1606	1007	276	319	4			
2	l	217	Total	C	N	O	S	0	0	0
			1606	1007	276	319	4			
2	n	217	Total	C	N	O	S	0	0	0
			1606	1007	276	319	4			
2	p	217	Total	C	N	O	S	0	0	0
			1606	1007	276	319	4			
2	r	217	Total	C	N	O	S	0	0	0
			1606	1007	276	319	4			
2	t	217	Total	C	N	O	S	0	0	0
			1606	1007	276	319	4			
2	v	219	Total	C	N	O	S	0	0	0
			1615	1012	278	321	4			
2	x	217	Total	C	N	O	S	0	0	0
			1606	1007	276	319	4			
2	z	217	Total	C	N	O	S	0	0	0
			1606	1007	276	319	4			
2	4	217	Total	C	N	O	S	0	0	0
			1606	1007	276	319	4			

There are 196 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	1	OZT	-	INSERTION	UNP O33245
H	235	HIS	-	EXPRESSION TAG	UNP O33245
H	236	HIS	-	EXPRESSION TAG	UNP O33245
H	237	HIS	-	EXPRESSION TAG	UNP O33245
H	238	HIS	-	EXPRESSION TAG	UNP O33245
H	239	HIS	-	EXPRESSION TAG	UNP O33245
H	240	HIS	-	EXPRESSION TAG	UNP O33245
C	1	OZT	-	INSERTION	UNP O33245
C	235	HIS	-	EXPRESSION TAG	UNP O33245

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	236	HIS	-	EXPRESSION TAG	UNP O33245
C	237	HIS	-	EXPRESSION TAG	UNP O33245
C	238	HIS	-	EXPRESSION TAG	UNP O33245
C	239	HIS	-	EXPRESSION TAG	UNP O33245
C	240	HIS	-	EXPRESSION TAG	UNP O33245
E	1	OZT	-	INSERTION	UNP O33245
E	235	HIS	-	EXPRESSION TAG	UNP O33245
E	236	HIS	-	EXPRESSION TAG	UNP O33245
E	237	HIS	-	EXPRESSION TAG	UNP O33245
E	238	HIS	-	EXPRESSION TAG	UNP O33245
E	239	HIS	-	EXPRESSION TAG	UNP O33245
E	240	HIS	-	EXPRESSION TAG	UNP O33245
G	1	OZT	-	INSERTION	UNP O33245
G	235	HIS	-	EXPRESSION TAG	UNP O33245
G	236	HIS	-	EXPRESSION TAG	UNP O33245
G	237	HIS	-	EXPRESSION TAG	UNP O33245
G	238	HIS	-	EXPRESSION TAG	UNP O33245
G	239	HIS	-	EXPRESSION TAG	UNP O33245
G	240	HIS	-	EXPRESSION TAG	UNP O33245
J	1	OZT	-	INSERTION	UNP O33245
J	235	HIS	-	EXPRESSION TAG	UNP O33245
J	236	HIS	-	EXPRESSION TAG	UNP O33245
J	237	HIS	-	EXPRESSION TAG	UNP O33245
J	238	HIS	-	EXPRESSION TAG	UNP O33245
J	239	HIS	-	EXPRESSION TAG	UNP O33245
J	240	HIS	-	EXPRESSION TAG	UNP O33245
L	1	OZT	-	INSERTION	UNP O33245
L	235	HIS	-	EXPRESSION TAG	UNP O33245
L	236	HIS	-	EXPRESSION TAG	UNP O33245
L	237	HIS	-	EXPRESSION TAG	UNP O33245
L	238	HIS	-	EXPRESSION TAG	UNP O33245
L	239	HIS	-	EXPRESSION TAG	UNP O33245
L	240	HIS	-	EXPRESSION TAG	UNP O33245
N	1	OZT	-	INSERTION	UNP O33245
N	235	HIS	-	EXPRESSION TAG	UNP O33245
N	236	HIS	-	EXPRESSION TAG	UNP O33245
N	237	HIS	-	EXPRESSION TAG	UNP O33245
N	238	HIS	-	EXPRESSION TAG	UNP O33245
N	239	HIS	-	EXPRESSION TAG	UNP O33245
N	240	HIS	-	EXPRESSION TAG	UNP O33245
P	1	OZT	-	INSERTION	UNP O33245
P	235	HIS	-	EXPRESSION TAG	UNP O33245

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
P	236	HIS	-	EXPRESSION TAG	UNP O33245
P	237	HIS	-	EXPRESSION TAG	UNP O33245
P	238	HIS	-	EXPRESSION TAG	UNP O33245
P	239	HIS	-	EXPRESSION TAG	UNP O33245
P	240	HIS	-	EXPRESSION TAG	UNP O33245
R	1	OZT	-	INSERTION	UNP O33245
R	235	HIS	-	EXPRESSION TAG	UNP O33245
R	236	HIS	-	EXPRESSION TAG	UNP O33245
R	237	HIS	-	EXPRESSION TAG	UNP O33245
R	238	HIS	-	EXPRESSION TAG	UNP O33245
R	239	HIS	-	EXPRESSION TAG	UNP O33245
R	240	HIS	-	EXPRESSION TAG	UNP O33245
T	1	OZT	-	INSERTION	UNP O33245
T	235	HIS	-	EXPRESSION TAG	UNP O33245
T	236	HIS	-	EXPRESSION TAG	UNP O33245
T	237	HIS	-	EXPRESSION TAG	UNP O33245
T	238	HIS	-	EXPRESSION TAG	UNP O33245
T	239	HIS	-	EXPRESSION TAG	UNP O33245
T	240	HIS	-	EXPRESSION TAG	UNP O33245
V	1	OZT	-	INSERTION	UNP O33245
V	235	HIS	-	EXPRESSION TAG	UNP O33245
V	236	HIS	-	EXPRESSION TAG	UNP O33245
V	237	HIS	-	EXPRESSION TAG	UNP O33245
V	238	HIS	-	EXPRESSION TAG	UNP O33245
V	239	HIS	-	EXPRESSION TAG	UNP O33245
V	240	HIS	-	EXPRESSION TAG	UNP O33245
X	1	OZT	-	INSERTION	UNP O33245
X	235	HIS	-	EXPRESSION TAG	UNP O33245
X	236	HIS	-	EXPRESSION TAG	UNP O33245
X	237	HIS	-	EXPRESSION TAG	UNP O33245
X	238	HIS	-	EXPRESSION TAG	UNP O33245
X	239	HIS	-	EXPRESSION TAG	UNP O33245
X	240	HIS	-	EXPRESSION TAG	UNP O33245
Z	1	OZT	-	INSERTION	UNP O33245
Z	235	HIS	-	EXPRESSION TAG	UNP O33245
Z	236	HIS	-	EXPRESSION TAG	UNP O33245
Z	237	HIS	-	EXPRESSION TAG	UNP O33245
Z	238	HIS	-	EXPRESSION TAG	UNP O33245
Z	239	HIS	-	EXPRESSION TAG	UNP O33245
Z	240	HIS	-	EXPRESSION TAG	UNP O33245
2	1	OZT	-	INSERTION	UNP O33245
2	235	HIS	-	EXPRESSION TAG	UNP O33245

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
2	236	HIS	-	EXPRESSION TAG	UNP O33245
2	237	HIS	-	EXPRESSION TAG	UNP O33245
2	238	HIS	-	EXPRESSION TAG	UNP O33245
2	239	HIS	-	EXPRESSION TAG	UNP O33245
2	240	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
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
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
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

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
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
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

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
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
4	301	OZT	-	INSERTION	UNP O33245
4	535	HIS	-	EXPRESSION TAG	UNP O33245
4	536	HIS	-	EXPRESSION TAG	UNP O33245
4	537	HIS	-	EXPRESSION TAG	UNP O33245
4	538	HIS	-	EXPRESSION TAG	UNP O33245
4	539	HIS	-	EXPRESSION TAG	UNP O33245
4	540	HIS	-	EXPRESSION TAG	UNP O33245

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	2	Total O 2 2	0	0
3	B	2	Total O 2 2	0	0
3	F	3	Total O 3 3	0	0
3	I	4	Total O 4 4	0	0
3	K	3	Total O 3 3	0	0
3	M	1	Total O 1 1	0	0
3	O	3	Total O 3 3	0	0
3	S	2	Total O 2 2	0	0
3	U	1	Total O 1 1	0	0
3	1	3	Total O 3 3	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	a	5	Total 5	O 5	0	0
3	b	3	Total 3	O 3	0	0
3	d	2	Total 2	O 2	0	0
3	f	1	Total 1	O 1	0	0
3	i	1	Total 1	O 1	0	0
3	k	2	Total 2	O 2	0	0
3	o	1	Total 1	O 1	0	0
3	q	1	Total 1	O 1	0	0
3	s	2	Total 2	O 2	0	0
3	u	2	Total 2	O 2	0	0
3	w	4	Total 4	O 4	0	0
3	y	2	Total 2	O 2	0	0
3	3	5	Total 5	O 5	0	0
3	H	1	Total 1	O 1	0	0
3	E	4	Total 4	O 4	0	0
3	G	2	Total 2	O 2	0	0
3	J	2	Total 2	O 2	0	0
3	L	1	Total 1	O 1	0	0
3	N	6	Total 6	O 6	0	0
3	P	4	Total 4	O 4	0	0
3	R	3	Total 3	O 3	0	0

Continued on next page...

Continued from previous page...

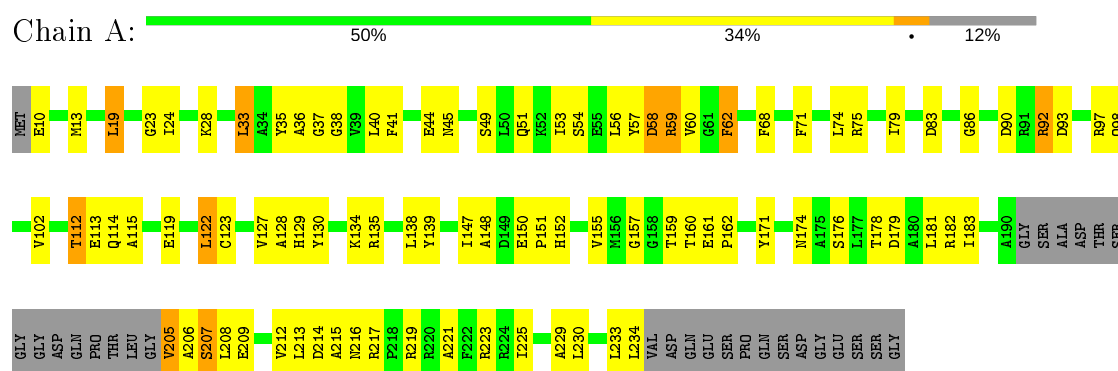
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	T	1	Total 1	O 1	0	0
3	V	6	Total 6	O 6	0	0
3	X	4	Total 4	O 4	0	0
3	2	1	Total 1	O 1	0	0
3	h	3	Total 3	O 3	0	0
3	c	6	Total 6	O 6	0	0
3	e	5	Total 5	O 5	0	0
3	g	3	Total 3	O 3	0	0
3	j	3	Total 3	O 3	0	0
3	l	3	Total 3	O 3	0	0
3	n	2	Total 2	O 2	0	0
3	p	2	Total 2	O 2	0	0
3	r	2	Total 2	O 2	0	0
3	t	2	Total 2	O 2	0	0
3	v	4	Total 4	O 4	0	0
3	x	1	Total 1	O 1	0	0
3	z	4	Total 4	O 4	0	0
3	4	7	Total 7	O 7	0	0

3 Residue-property plots

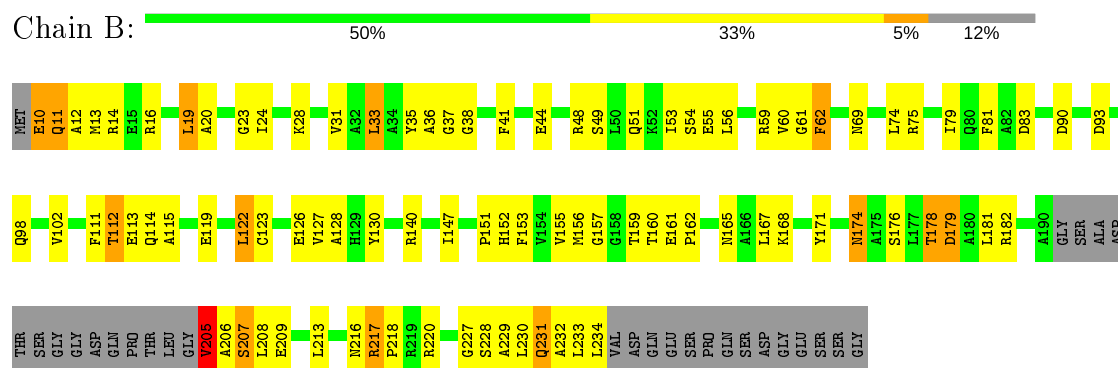
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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.

Note EDS failed to run properly.

• Molecule 1: Proteasome (Alpha subunit) PrcA

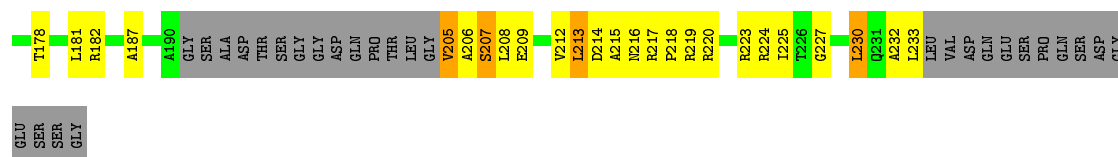


• Molecule 1: Proteasome (Alpha subunit) PrcA

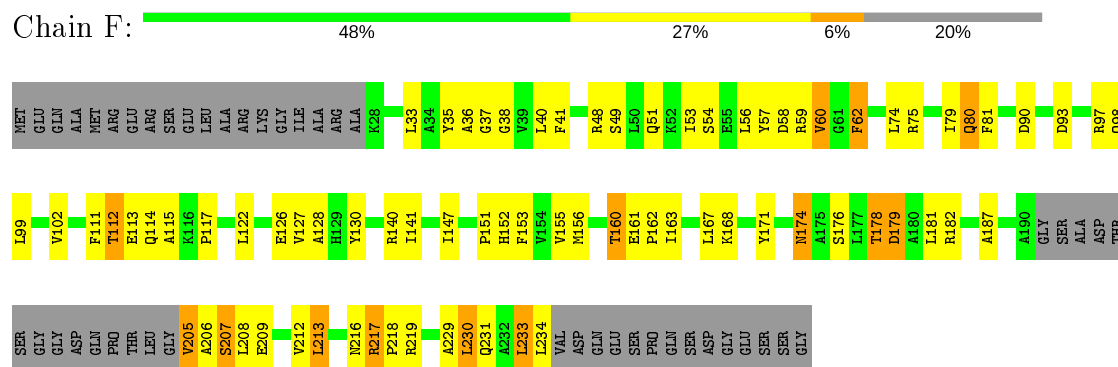


• Molecule 1: Proteasome (Alpha subunit) PrcA

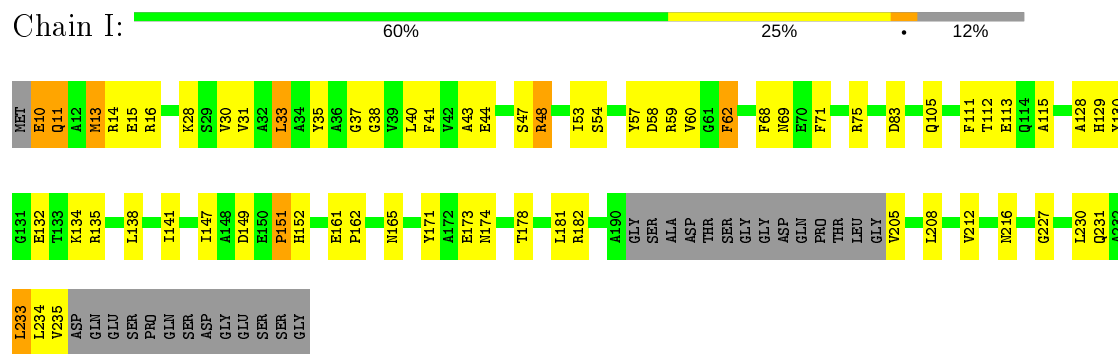




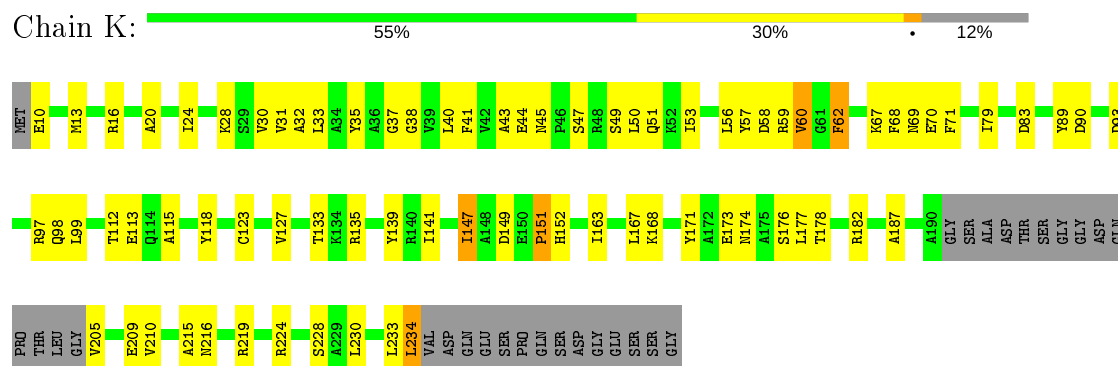
• Molecule 1: Proteasome (Alpha subunit) PrcA



• Molecule 1: Proteasome (Alpha subunit) PrcA

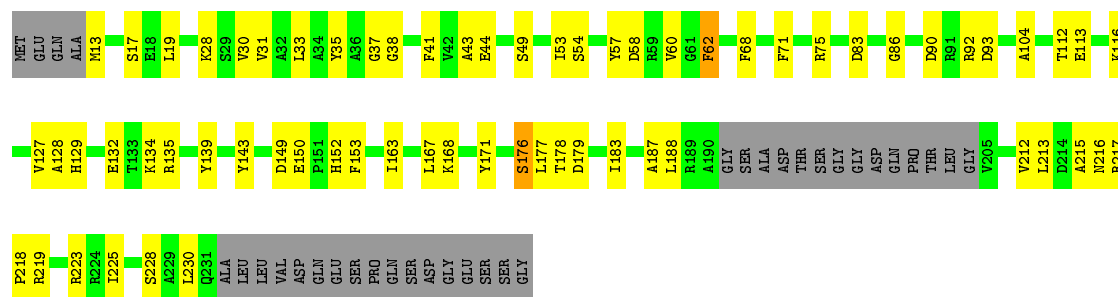


• Molecule 1: Proteasome (Alpha subunit) PrcA



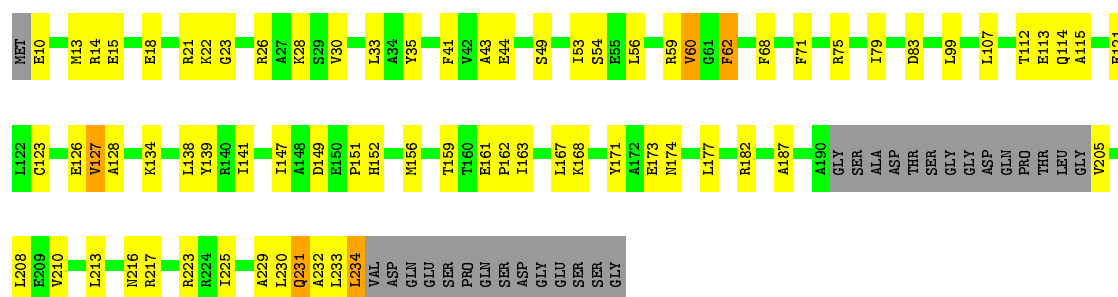
• Molecule 1: Proteasome (Alpha subunit) PrcA



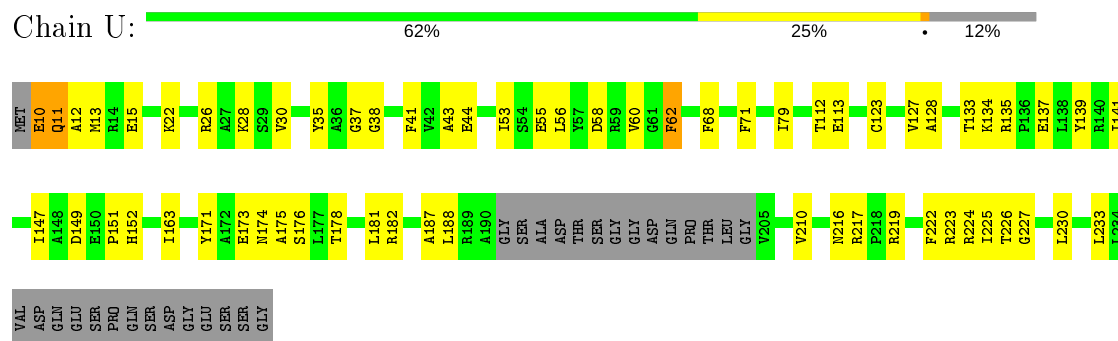


• Molecule 1: Proteasome (Alpha subunit) PrcA

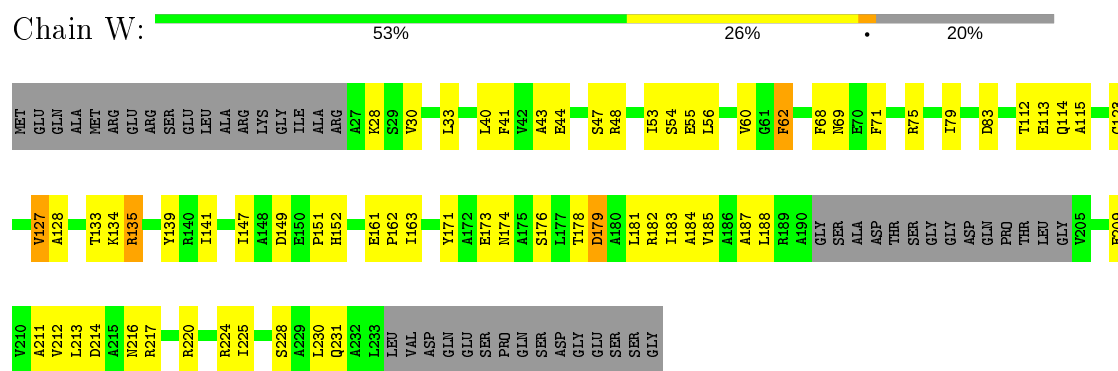
Chain O: 57% 29% 12%



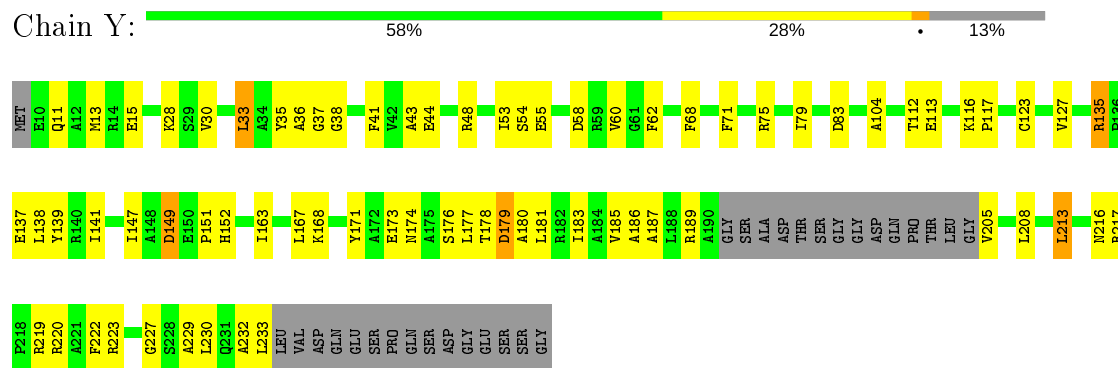
- Molecule 1: Proteasome (Alpha subunit) PrcA



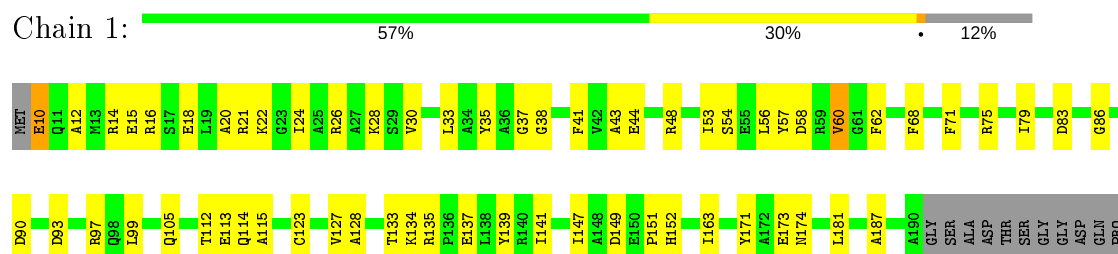
- Molecule 1: Proteasome (Alpha subunit) PrcA



- Molecule 1: Proteasome (Alpha subunit) PrcA

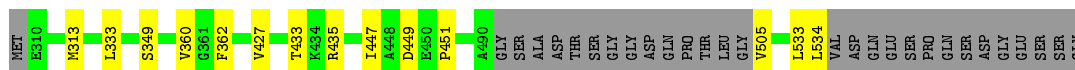
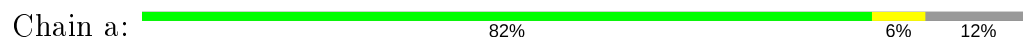


- Molecule 1: Proteasome (Alpha subunit) PrcA

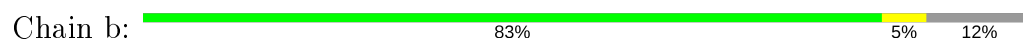




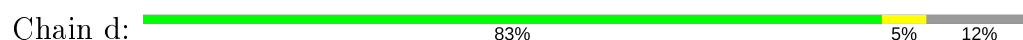
- Molecule 1: Proteasome (Alpha subunit) PrcA



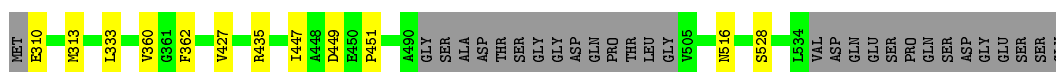
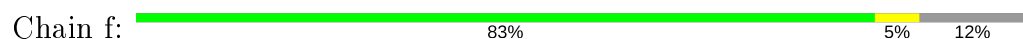
- Molecule 1: Proteasome (Alpha subunit) PrcA



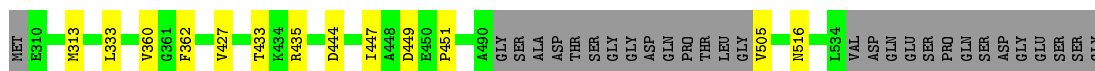
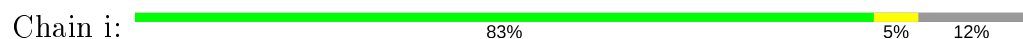
- Molecule 1: Proteasome (Alpha subunit) PrcA



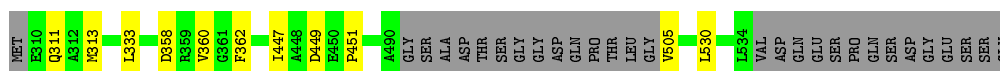
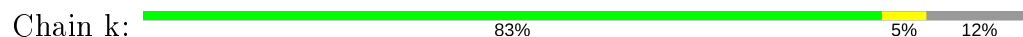
- Molecule 1: Proteasome (Alpha subunit) PrcA



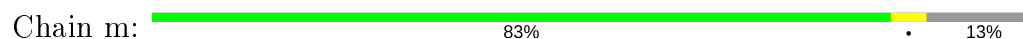
- Molecule 1: Proteasome (Alpha subunit) PrcA

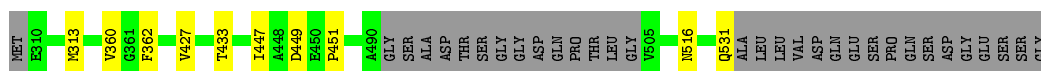


- Molecule 1: Proteasome (Alpha subunit) PrcA

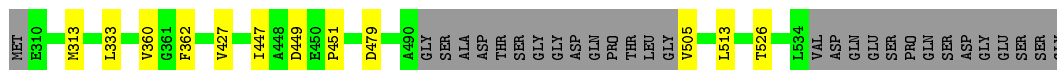
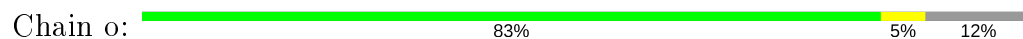


- Molecule 1: Proteasome (Alpha subunit) PrcA

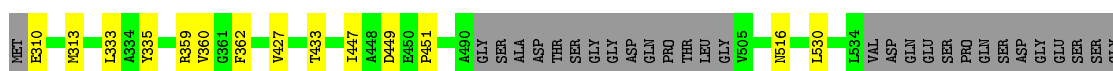
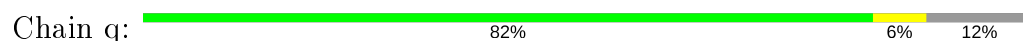




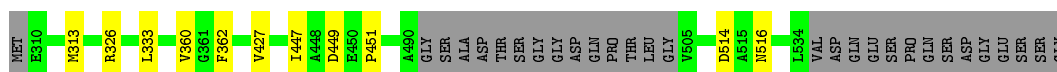
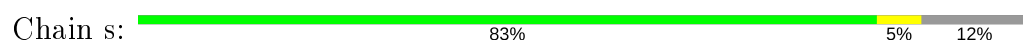
- Molecule 1: Proteasome (Alpha subunit) PrcA



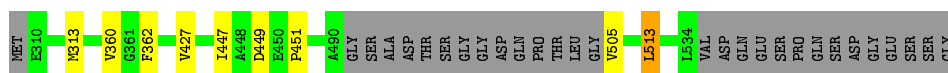
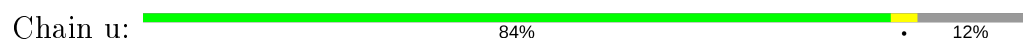
- Molecule 1: Proteasome (Alpha subunit) PrcA



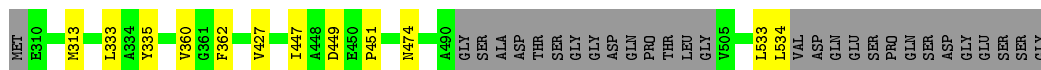
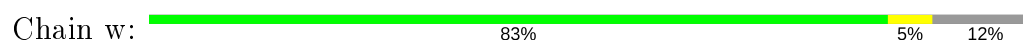
- Molecule 1: Proteasome (Alpha subunit) PrcA



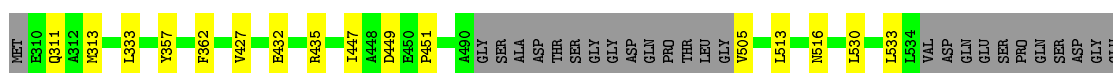
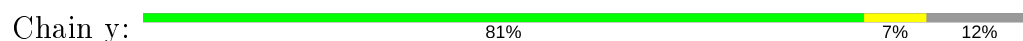
- Molecule 1: Proteasome (Alpha subunit) PrcA



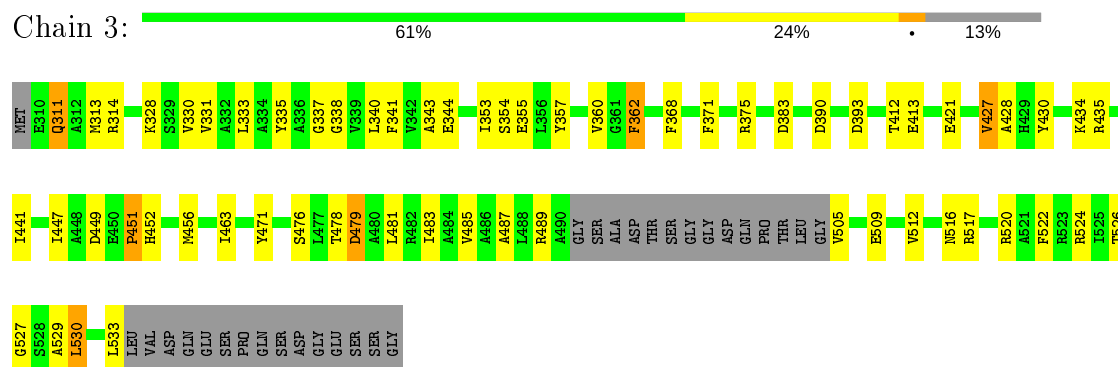
- Molecule 1: Proteasome (Alpha subunit) PrcA



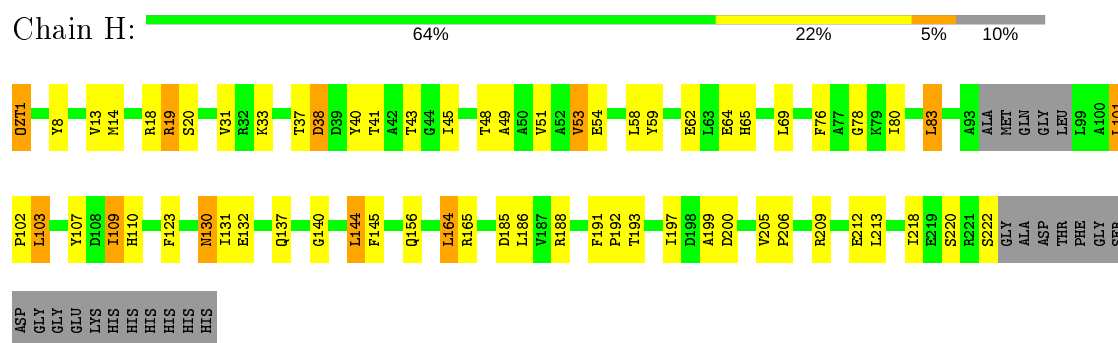
- Molecule 1: Proteasome (Alpha subunit) PrcA



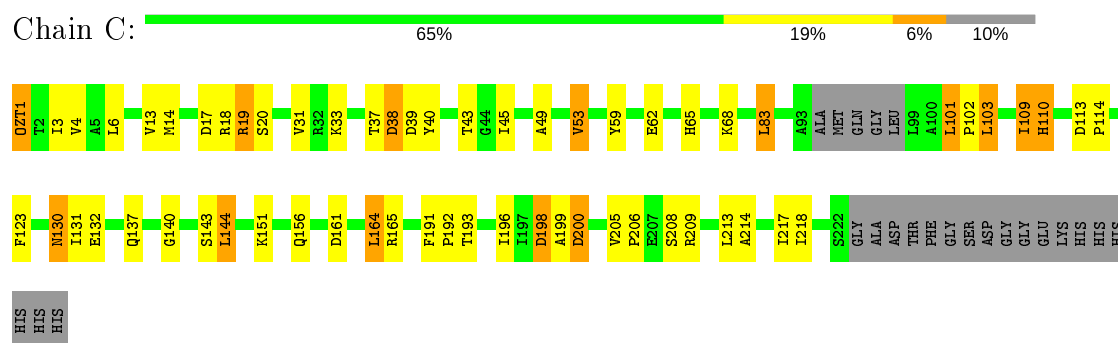
- Molecule 1: Proteasome (Alpha subunit) PrcA



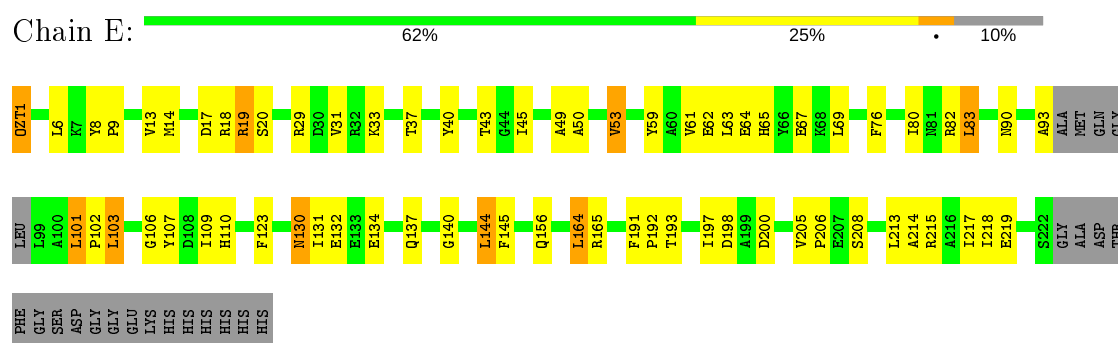
- Molecule 2: Proteasome (Beta subunit) PrcB



- Molecule 2: Proteasome (Beta subunit) PrcB

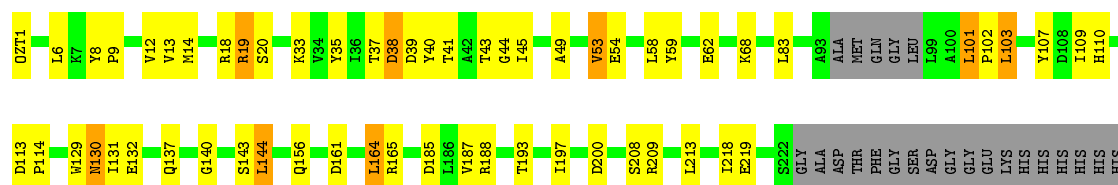


- Molecule 2: Proteasome (Beta subunit) PrcB



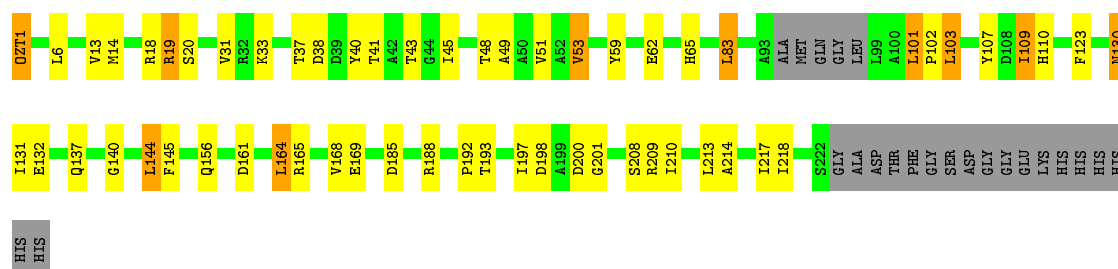
- Molecule 2: Proteasome (Beta subunit) PrCB

Chain G:  66% 21% 10%



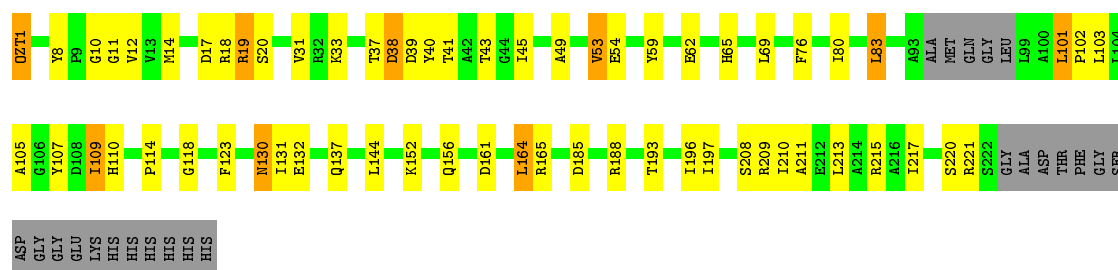
• Molecule 2: Proteasome (Beta subunit) PrcB

Chain J:  66% 20% 10%



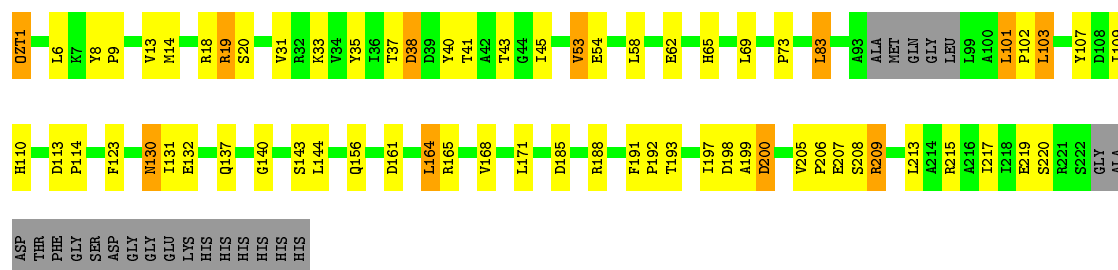
• Molecule 2: Proteasome (Beta subunit) PrcB

Chain L:  64% 23% 10%



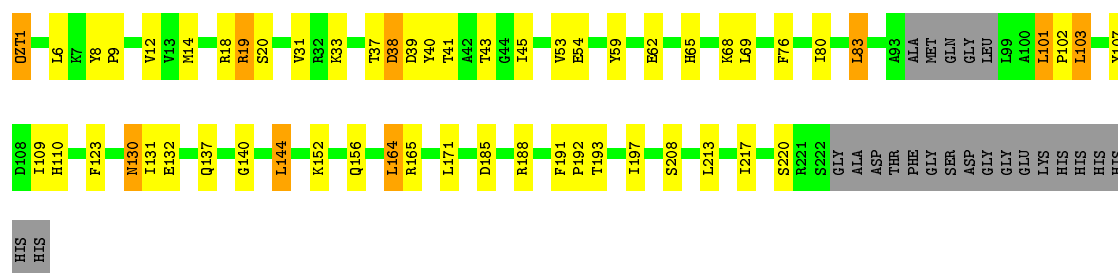
• Molecule 2: Proteasome (Beta subunit) PrcB

Chain N:  63% 23% 5% 10%

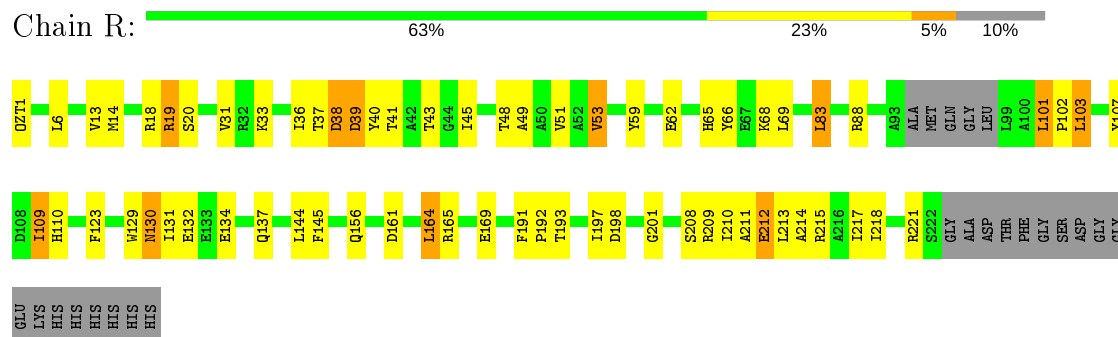


• Molecule 2: Proteasome (Beta subunit) PrcB

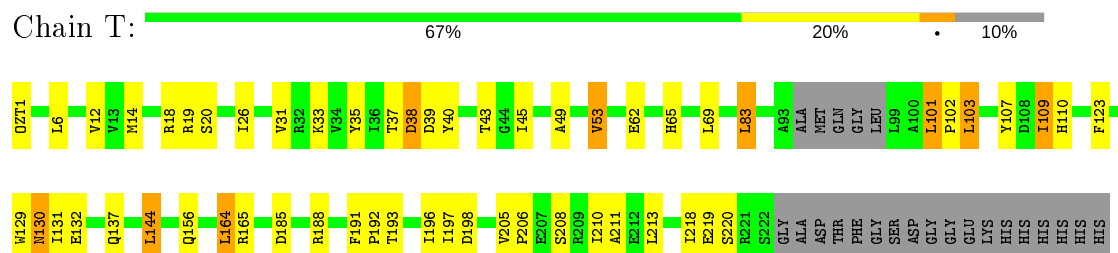
Chain P:  67% 20% 10%



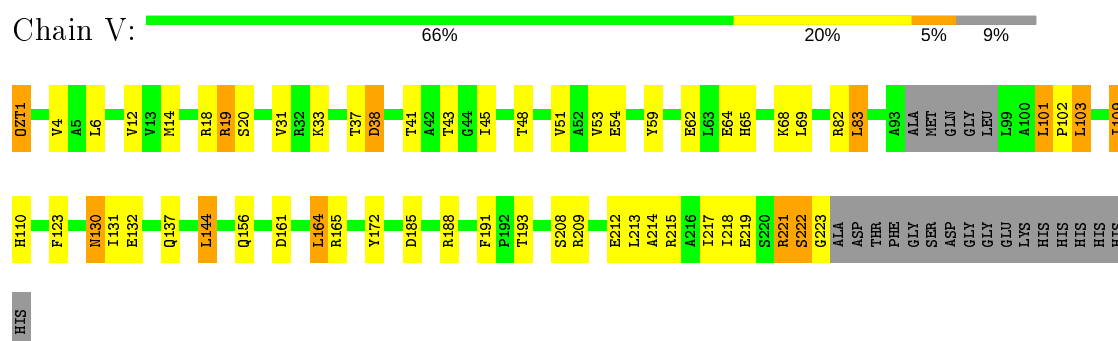
- Molecule 2: Proteasome (Beta subunit) PrcB



- Molecule 2: Proteasome (Beta subunit) PrcB



- Molecule 2: Proteasome (Beta subunit) PrcB




- Molecule 2: Proteasome (Beta subunit) PrcB




HIS
HIS

• Molecule 2: Proteasome (Beta subunit) PrcB

Chain e:  84% 6% 10%


O2T301	R319	V353	E362	L383	A393	ALA	MET	GLN	GLY	LEU	L399	A400	L401	P402	L403	I409	H410	N430	L444	L464	D500	S508	S520	R521	S522	GLY	ALA	ASP	THR	PHE	GLY	SER	ASP	GLY	GLY	LYS	HIS	HIS	HIS	HIS	HIS	HIS
--------	------	------	------	------	------	-----	-----	-----	-----	-----	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

• Molecule 2: Proteasome (Beta subunit) PrcB

Chain g:  84% 6% 10%

O2T301	V304	R319	V353	E362	L383	A393	ALA	MET	GLN	GLY	LEU	L399	A400	P402	L403	I409	H410	N430	L444	L464	S508	R509	S522	GLY	ALA	ASP	THR	PHE	GLY	SER	ASP	GLY	GLY	LYS	HIS	HIS	HIS	HIS	HIS	HIS
--------	------	------	------	------	------	------	-----	-----	-----	-----	-----	------	------	------	------	------	------	------	------	------	------	------	------	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----


• Molecule 2: Proteasome (Beta subunit) PrcB

Chain j:  83% 8% 10%

O2T301	V304	V312	R319	V353	E362	L383	A393	ALA	MET	GLN	GLY	LEU	L399	A400	L401	P402	L403	I409	H410	N430	L444	D461	L464	I496	B517	S520	R521	S522	GLY	ALA	ASP	THR	PHE	GLY	GLY	LYS	HIS	HIS	HIS	HIS	HIS
--------	------	------	------	------	------	------	------	-----	-----	-----	-----	-----	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----


HIS
HIS

• Molecule 2: Proteasome (Beta subunit) PrcB

Chain l:  84% 7% 10%


O2T301	R319	V353	E362	L383	A393	ALA	MET	GLN	GLY	LEU	L399	A400	L401	P402	L403	I409	H410	N430	L444	L464	I496	S508	E512	S520	R521	S522	GLY	ALA	ASP	THR	PHE	GLY	GLY	LYS	HIS	HIS	HIS	HIS	HIS	HIS
--------	------	------	------	------	------	-----	-----	-----	-----	-----	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

• Molecule 2: Proteasome (Beta subunit) PrcB

Chain n:  83% 7% 10%


O2T301	V312	R319	D339	V353	E362	L383	A393	ALA	MET	GLN	GLY	LEU	L399	A400	L401	P402	L403	N430	L444	D461	L464	I496	S508	S520	R521	S522	GLY	ALA	ASP	THR	PHE	GLY	GLY	LYS	HIS	HIS	HIS	HIS	HIS	HIS
--------	------	------	------	------	------	------	------	-----	-----	-----	-----	-----	------	------	------	------	------	------	------	------	------	------	------	------	------	------	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

• Molecule 2: Proteasome (Beta subunit) PrcB

Chain p:  85% 6% 10%


O2T301	V353	E362	L383	A393	ALA	MET	GLN	GLY	LEU	L399	A400	L401	P402	L403	I409	H410	N430	L444	L464	I496	D500	S508	S522	GLY	ALA	ASP	THR	PHE	GLY	GLY	LYS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS
--------	------	------	------	------	-----	-----	-----	-----	-----	------	------	------	------	------	------	------	------	------	------	------	------	------	------	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

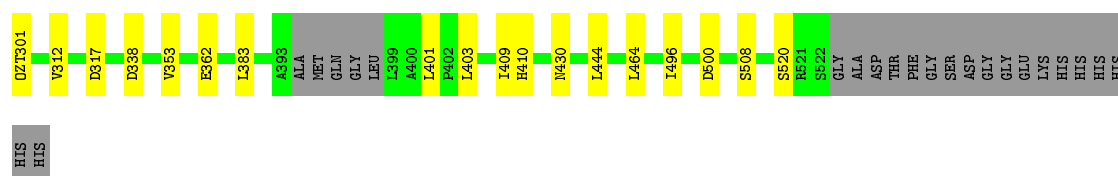
- Molecule 2: Proteasome (Beta subunit) PrcB

Chain r:  85% 6% 10%




- Molecule 2: Proteasome (Beta subunit) PrcB

Chain t:  83% 8% 10%




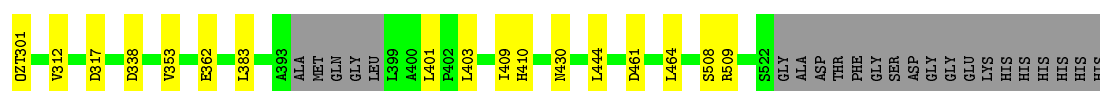
- Molecule 2: Proteasome (Beta subunit) PrcB

Chain v:  84% 7% 9%




- Molecule 2: Proteasome (Beta subunit) PrcB

Chain x:  83% 7% 10%



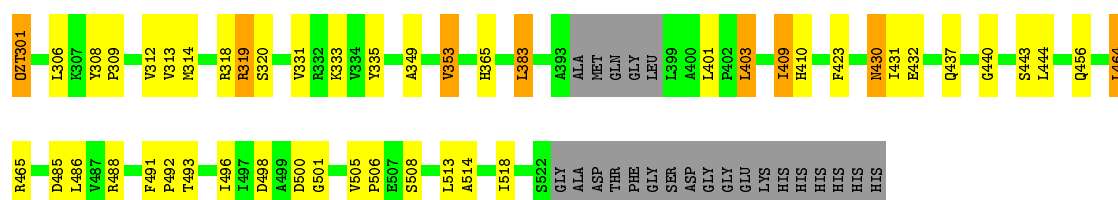
- Molecule 2: Proteasome (Beta subunit) PrcB

Chain z:  84% 7% 10%



- Molecule 2: Proteasome (Beta subunit) PrcB

Chain 4:  70% 17% 10%



4 Data and refinement statistics

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	119.58Å 209.62Å 284.93Å 90.00° 102.01° 90.00°	Depositor
Resolution (Å)	25.12 – 2.88	Depositor
% Data completeness (in resolution range)	88.6 (25.12-2.88)	Depositor
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.16 (at 2.89Å)	Xtriage
Refinement program	PHENIX (phenix.refine), CNS	Depositor
R, R_{free}	0.217 , 0.267	Depositor
Wilson B-factor (Å ²)	35.8	Xtriage
Anisotropy	0.140	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.000 for h,-k,-h-l	Xtriage
Total number of atoms	90443	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 57.88 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.2193e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	1	0.50	0/1657	0.63	0/2238
1	3	0.52	0/1649	0.64	0/2227
1	A	0.55	0/1657	0.71	2/2238 (0.1%)
1	B	0.62	2/1657 (0.1%)	0.72	1/2238 (0.0%)
1	D	0.44	0/1649	0.63	0/2227
1	F	0.57	0/1514	0.71	0/2050
1	I	0.50	0/1664	0.65	0/2248
1	K	0.49	0/1657	0.68	0/2238
1	M	0.48	0/1613	0.65	0/2178
1	O	0.53	0/1657	0.67	1/2238 (0.0%)
1	Q	0.43	0/1657	0.62	0/2238
1	S	0.50	0/1657	0.65	0/2238
1	U	0.49	0/1657	0.62	0/2238
1	W	0.43	0/1511	0.60	0/2046
1	Y	0.48	0/1649	0.65	1/2227 (0.0%)
1	a	0.52	0/1657	0.65	0/2238
1	b	0.56	0/1657	0.67	0/2238
1	d	0.44	0/1657	0.61	0/2238
1	f	0.48	0/1657	0.60	0/2238
1	i	0.53	0/1657	0.64	0/2238
1	k	0.48	0/1657	0.64	0/2238
1	m	0.47	0/1636	0.62	0/2209
1	o	0.48	0/1657	0.62	0/2238
1	q	0.45	0/1657	0.61	0/2238
1	s	0.51	0/1657	0.65	1/2238 (0.0%)
1	u	0.48	0/1657	0.63	1/2238 (0.0%)
1	w	0.45	0/1657	0.60	0/2238
1	y	0.45	0/1657	0.62	0/2238
2	2	0.63	0/1620	0.70	0/2196
2	4	0.62	0/1620	0.69	0/2196
2	C	0.56	0/1620	0.68	0/2196
2	E	0.53	0/1620	0.66	0/2196

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
2	G	0.64	0/1620	0.69	0/2196
2	H	0.62	0/1620	0.69	0/2196
2	J	0.55	0/1620	0.65	0/2196
2	L	0.63	0/1620	0.69	0/2196
2	N	0.70	0/1620	0.74	0/2196
2	P	0.73	0/1620	0.74	0/2196
2	R	0.52	0/1620	0.65	0/2196
2	T	0.61	0/1620	0.70	0/2196
2	V	0.69	0/1624	0.70	0/2201
2	X	0.65	0/1620	0.71	0/2196
2	Z	0.55	0/1620	0.67	0/2196
2	c	0.58	0/1610	0.68	0/2182
2	e	0.59	0/1620	0.70	0/2196
2	g	0.64	0/1620	0.69	0/2196
2	h	0.65	0/1602	0.71	1/2171 (0.0%)
2	j	0.57	0/1620	0.67	0/2196
2	l	0.63	0/1620	0.71	0/2196
2	n	0.67	0/1620	0.72	0/2196
2	p	0.71	0/1620	0.72	0/2196
2	r	0.56	0/1620	0.67	0/2196
2	t	0.58	0/1620	0.66	0/2196
2	v	0.67	0/1629	0.71	0/2208
2	x	0.60	0/1620	0.68	0/2196
2	z	0.52	0/1620	0.65	0/2196
All	All	0.56	2/91370 (0.0%)	0.67	8/123638 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	123	CYS	CB-SG	-5.97	1.72	1.81
1	B	205	VAL	CB-CG1	5.49	1.64	1.52

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	19	LEU	CA-CB-CG	5.99	129.08	115.30
1	A	92	ARG	NE-CZ-NH2	-5.50	117.55	120.30
2	h	353	VAL	CB-CA-C	-5.33	101.28	111.40
1	O	213	LEU	N-CA-C	-5.20	96.95	111.00
1	u	513	LEU	N-CA-C	-5.20	96.96	111.00

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	1633	0	1633	66	0
1	3	1625	0	1622	57	0
1	A	1633	0	1633	101	0
1	B	1633	0	1633	86	0
1	D	1625	0	1622	145	0
1	F	1490	0	1483	76	0
1	I	1640	0	1642	90	0
1	K	1633	0	1633	70	0
1	M	1589	0	1587	75	0
1	O	1633	0	1633	54	0
1	Q	1633	0	1633	85	0
1	S	1633	0	1633	98	0
1	U	1633	0	1633	54	0
1	W	1487	0	1477	64	0
1	Y	1625	0	1622	91	0
1	a	1633	0	1633	0	0
1	b	1633	0	1633	0	0
1	d	1633	0	1633	0	0
1	f	1633	0	1633	0	0
1	i	1633	0	1633	0	0
1	k	1633	0	1633	0	0
1	m	1612	0	1606	0	0
1	o	1633	0	1633	0	0
1	q	1633	0	1633	0	0
1	s	1633	0	1633	0	0
1	u	1633	0	1633	0	0
1	w	1633	0	1633	0	0
1	y	1633	0	1633	0	0
2	2	1606	0	1593	46	0
2	4	1606	0	1593	35	0
2	C	1606	0	1593	46	0
2	E	1606	0	1593	69	0
2	G	1606	0	1593	46	0
2	H	1606	0	1593	58	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	J	1606	0	1593	49	0
2	L	1606	0	1593	55	0
2	N	1606	0	1593	44	0
2	P	1606	0	1593	40	0
2	R	1606	0	1593	69	0
2	T	1606	0	1593	43	0
2	V	1610	0	1596	64	0
2	X	1606	0	1593	57	0
2	Z	1606	0	1593	56	0
2	c	1596	0	1583	0	0
2	e	1606	0	1593	0	0
2	g	1606	0	1593	0	0
2	h	1588	0	1572	0	0
2	j	1606	0	1593	0	0
2	l	1606	0	1593	0	0
2	n	1606	0	1593	0	0
2	p	1606	0	1593	0	0
2	r	1606	0	1593	0	0
2	t	1606	0	1593	0	0
2	v	1615	0	1601	0	0
2	x	1606	0	1593	0	0
2	z	1606	0	1593	0	0
3	1	3	0	0	1	0
3	2	1	0	0	0	0
3	3	5	0	0	2	0
3	4	7	0	0	1	0
3	A	2	0	0	2	0
3	B	2	0	0	1	0
3	E	4	0	0	2	0
3	F	3	0	0	2	0
3	G	2	0	0	1	0
3	H	1	0	0	1	0
3	I	4	0	0	3	0
3	J	2	0	0	0	0
3	K	3	0	0	4	0
3	L	1	0	0	0	0
3	M	1	0	0	1	0
3	N	6	0	0	4	0
3	O	3	0	0	1	0
3	P	4	0	0	0	0
3	R	3	0	0	2	0
3	S	2	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	T	1	0	0	1	0
3	U	1	0	0	0	0
3	V	6	0	0	0	0
3	X	4	0	0	0	0
3	a	5	0	0	0	0
3	b	3	0	0	0	0
3	c	6	0	0	0	0
3	d	2	0	0	0	0
3	e	5	0	0	0	0
3	f	1	0	0	0	0
3	g	3	0	0	0	0
3	h	3	0	0	0	0
3	i	1	0	0	0	0
3	j	3	0	0	0	0
3	k	2	0	0	0	0
3	l	3	0	0	0	0
3	n	2	0	0	0	0
3	o	1	0	0	0	0
3	p	2	0	0	0	0
3	q	1	0	0	0	0
3	r	2	0	0	0	0
3	s	2	0	0	0	0
3	t	2	0	0	0	0
3	u	2	0	0	0	0
3	v	4	0	0	0	0
3	w	4	0	0	0	0
3	x	1	0	0	0	0
3	y	2	0	0	0	0
3	z	4	0	0	0	0
All	All	90443	0	89905	1864	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 19.

The worst 5 of 1864 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:35:TYR:CE2	1:D:40:LEU:HB2	1.65	1.32
1:M:35:TYR:CE1	1:M:37:GLY:HA3	1.68	1.26
1:S:230:LEU:C	1:S:230:LEU:HD23	1.51	1.21
1:B:19:LEU:HD23	1:B:19:LEU:C	1.61	1.18

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:229:ALA:O	1:1:233:LEU:HD13	1.41	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	207/240 (86%)	193 (93%)	13 (6%)	1 (0%)	29	59
1	3	206/240 (86%)	196 (95%)	9 (4%)	1 (0%)	29	59
1	A	207/240 (86%)	189 (91%)	18 (9%)	0	100	100
1	B	207/240 (86%)	187 (90%)	19 (9%)	1 (0%)	29	59
1	D	206/240 (86%)	185 (90%)	21 (10%)	0	100	100
1	F	189/240 (79%)	170 (90%)	18 (10%)	1 (0%)	29	59
1	I	208/240 (87%)	199 (96%)	8 (4%)	1 (0%)	29	59
1	K	207/240 (86%)	196 (95%)	10 (5%)	1 (0%)	29	59
1	M	201/240 (84%)	190 (94%)	11 (6%)	0	100	100
1	O	207/240 (86%)	197 (95%)	9 (4%)	1 (0%)	29	59
1	Q	207/240 (86%)	194 (94%)	12 (6%)	1 (0%)	29	59
1	S	207/240 (86%)	194 (94%)	12 (6%)	1 (0%)	29	59
1	U	207/240 (86%)	194 (94%)	12 (6%)	1 (0%)	29	59
1	W	189/240 (79%)	175 (93%)	13 (7%)	1 (0%)	29	59
1	Y	206/240 (86%)	196 (95%)	9 (4%)	1 (0%)	29	59
1	a	207/240 (86%)	197 (95%)	9 (4%)	1 (0%)	29	59
1	b	207/240 (86%)	193 (93%)	13 (6%)	1 (0%)	29	59
1	d	207/240 (86%)	196 (95%)	10 (5%)	1 (0%)	29	59
1	f	207/240 (86%)	190 (92%)	16 (8%)	1 (0%)	29	59

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	i	207/240 (86%)	195 (94%)	11 (5%)	1 (0%)	29	59
1	k	207/240 (86%)	199 (96%)	7 (3%)	1 (0%)	29	59
1	m	204/240 (85%)	190 (93%)	13 (6%)	1 (0%)	29	59
1	o	207/240 (86%)	194 (94%)	12 (6%)	1 (0%)	29	59
1	q	207/240 (86%)	194 (94%)	12 (6%)	1 (0%)	29	59
1	s	207/240 (86%)	196 (95%)	10 (5%)	1 (0%)	29	59
1	u	207/240 (86%)	198 (96%)	8 (4%)	1 (0%)	29	59
1	w	207/240 (86%)	197 (95%)	9 (4%)	1 (0%)	29	59
1	y	207/240 (86%)	197 (95%)	9 (4%)	1 (0%)	29	59
2	2	213/240 (89%)	208 (98%)	5 (2%)	0	100	100
2	4	213/240 (89%)	211 (99%)	2 (1%)	0	100	100
2	C	213/240 (89%)	212 (100%)	1 (0%)	0	100	100
2	E	213/240 (89%)	212 (100%)	1 (0%)	0	100	100
2	G	213/240 (89%)	209 (98%)	4 (2%)	0	100	100
2	H	213/240 (89%)	210 (99%)	3 (1%)	0	100	100
2	J	213/240 (89%)	211 (99%)	2 (1%)	0	100	100
2	L	213/240 (89%)	207 (97%)	6 (3%)	0	100	100
2	N	213/240 (89%)	210 (99%)	3 (1%)	0	100	100
2	P	213/240 (89%)	208 (98%)	5 (2%)	0	100	100
2	R	213/240 (89%)	209 (98%)	4 (2%)	0	100	100
2	T	213/240 (89%)	208 (98%)	5 (2%)	0	100	100
2	V	214/240 (89%)	209 (98%)	5 (2%)	0	100	100
2	X	213/240 (89%)	209 (98%)	4 (2%)	0	100	100
2	Z	213/240 (89%)	208 (98%)	5 (2%)	0	100	100
2	c	211/240 (88%)	205 (97%)	6 (3%)	0	100	100
2	e	213/240 (89%)	209 (98%)	4 (2%)	0	100	100
2	g	213/240 (89%)	206 (97%)	7 (3%)	0	100	100
2	h	210/240 (88%)	207 (99%)	3 (1%)	0	100	100
2	j	213/240 (89%)	207 (97%)	5 (2%)	1 (0%)	29	59
2	l	213/240 (89%)	209 (98%)	4 (2%)	0	100	100
2	n	213/240 (89%)	207 (97%)	6 (3%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	p	213/240 (89%)	205 (96%)	8 (4%)	0	100	100
2	r	213/240 (89%)	208 (98%)	5 (2%)	0	100	100
2	t	213/240 (89%)	211 (99%)	2 (1%)	0	100	100
2	v	215/240 (90%)	212 (99%)	3 (1%)	0	100	100
2	x	213/240 (89%)	209 (98%)	4 (2%)	0	100	100
2	z	213/240 (89%)	211 (99%)	2 (1%)	0	100	100
All	All	11711/13440 (87%)	11238 (96%)	447 (4%)	26 (0%)	47	76

5 of 26 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	151	PRO
1	F	151	PRO
1	I	151	PRO
1	b	451	PRO
1	o	451	PRO

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	162/184 (88%)	151 (93%)	11 (7%)	16	40
1	3	161/184 (88%)	150 (93%)	11 (7%)	16	40
1	A	162/184 (88%)	149 (92%)	13 (8%)	12	32
1	B	162/184 (88%)	141 (87%)	21 (13%)	4	11
1	D	161/184 (88%)	143 (89%)	18 (11%)	6	16
1	F	149/184 (81%)	132 (89%)	17 (11%)	5	16
1	I	163/184 (89%)	150 (92%)	13 (8%)	12	32
1	K	162/184 (88%)	149 (92%)	13 (8%)	12	32
1	M	158/184 (86%)	151 (96%)	7 (4%)	28	59
1	O	162/184 (88%)	151 (93%)	11 (7%)	16	40

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	Q	162/184 (88%)	150 (93%)	12 (7%)	13	36
1	S	162/184 (88%)	150 (93%)	12 (7%)	13	36
1	U	162/184 (88%)	151 (93%)	11 (7%)	16	40
1	W	148/184 (80%)	139 (94%)	9 (6%)	18	45
1	Y	161/184 (88%)	149 (92%)	12 (8%)	13	35
1	a	162/184 (88%)	149 (92%)	13 (8%)	12	32
1	b	162/184 (88%)	150 (93%)	12 (7%)	13	36
1	d	162/184 (88%)	150 (93%)	12 (7%)	13	36
1	f	162/184 (88%)	151 (93%)	11 (7%)	16	40
1	i	162/184 (88%)	150 (93%)	12 (7%)	13	36
1	k	162/184 (88%)	152 (94%)	10 (6%)	18	45
1	m	160/184 (87%)	151 (94%)	9 (6%)	21	49
1	o	162/184 (88%)	151 (93%)	11 (7%)	16	40
1	q	162/184 (88%)	149 (92%)	13 (8%)	12	32
1	s	162/184 (88%)	153 (94%)	9 (6%)	21	49
1	u	162/184 (88%)	154 (95%)	8 (5%)	25	55
1	w	162/184 (88%)	151 (93%)	11 (7%)	16	40
1	y	162/184 (88%)	147 (91%)	15 (9%)	9	25
2	2	161/177 (91%)	147 (91%)	14 (9%)	10	28
2	4	161/177 (91%)	148 (92%)	13 (8%)	11	31
2	C	161/177 (91%)	146 (91%)	15 (9%)	9	25
2	E	161/177 (91%)	149 (92%)	12 (8%)	13	35
2	G	161/177 (91%)	146 (91%)	15 (9%)	9	25
2	H	161/177 (91%)	144 (89%)	17 (11%)	6	19
2	J	161/177 (91%)	149 (92%)	12 (8%)	13	35
2	L	161/177 (91%)	143 (89%)	18 (11%)	6	16
2	N	161/177 (91%)	144 (89%)	17 (11%)	6	19
2	P	161/177 (91%)	146 (91%)	15 (9%)	9	25
2	R	161/177 (91%)	146 (91%)	15 (9%)	9	25
2	T	161/177 (91%)	146 (91%)	15 (9%)	9	25
2	V	161/177 (91%)	143 (89%)	18 (11%)	6	16

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	X	161/177 (91%)	147 (91%)	14 (9%)	10	28
2	Z	161/177 (91%)	147 (91%)	14 (9%)	10	28
2	c	161/177 (91%)	145 (90%)	16 (10%)	8	22
2	e	161/177 (91%)	147 (91%)	14 (9%)	10	28
2	g	161/177 (91%)	147 (91%)	14 (9%)	10	28
2	h	160/177 (90%)	145 (91%)	15 (9%)	8	24
2	j	161/177 (91%)	145 (90%)	16 (10%)	8	22
2	l	161/177 (91%)	146 (91%)	15 (9%)	9	25
2	n	161/177 (91%)	145 (90%)	16 (10%)	8	22
2	p	161/177 (91%)	148 (92%)	13 (8%)	11	31
2	r	161/177 (91%)	148 (92%)	13 (8%)	11	31
2	t	161/177 (91%)	144 (89%)	17 (11%)	6	19
2	v	161/177 (91%)	145 (90%)	16 (10%)	8	22
2	x	161/177 (91%)	145 (90%)	16 (10%)	8	22
2	z	161/177 (91%)	146 (91%)	15 (9%)	9	25
All	All	9008/10108 (89%)	8251 (92%)	757 (8%)	11	30

5 of 757 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	H	101	LEU
2	L	209	ARG
2	v	338	ASP
2	H	220	SER
2	G	53	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 137 such sidechains are listed below:

Mol	Chain	Res	Type
1	o	414	GLN
1	3	398	GLN
2	t	365	HIS
1	q	414	GLN
1	u	452	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

28 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	J	1	2	7,9,10	2.92	2 (28%)	9,12,14	2.60	3 (33%)
2	OZT	2	1	2	7,9,10	2.65	2 (28%)	9,12,14	2.58	6 (66%)
2	OZT	4	301	2	7,9,10	3.07	2 (28%)	9,12,14	3.13	4 (44%)
2	OZT	Z	1	2	7,9,10	2.78	3 (42%)	9,12,14	2.60	3 (33%)
2	OZT	n	301	2	7,9,10	3.04	2 (28%)	9,12,14	2.34	4 (44%)
2	OZT	l	301	2	7,9,10	2.58	2 (28%)	9,12,14	2.46	4 (44%)
2	OZT	z	301	2	7,9,10	3.14	2 (28%)	9,12,14	3.22	4 (44%)
2	OZT	H	1	2	7,9,10	3.02	2 (28%)	9,12,14	2.38	4 (44%)
2	OZT	v	301	2	7,9,10	3.09	3 (42%)	9,12,14	3.30	4 (44%)
2	OZT	r	301	2	7,9,10	2.84	2 (28%)	9,12,14	3.09	4 (44%)
2	OZT	c	301	2	7,9,10	2.83	2 (28%)	9,12,14	2.70	6 (66%)
2	OZT	G	1	2	7,9,10	2.81	3 (42%)	9,12,14	2.74	3 (33%)
2	OZT	e	301	2	7,9,10	2.87	2 (28%)	9,12,14	2.22	5 (55%)
2	OZT	g	301	2	7,9,10	2.67	2 (28%)	9,12,14	2.53	5 (55%)
2	OZT	j	301	2	7,9,10	2.77	2 (28%)	9,12,14	2.12	5 (55%)
2	OZT	V	1	2	7,9,10	2.89	2 (28%)	9,12,14	2.19	4 (44%)
2	OZT	x	301	2	7,9,10	3.15	2 (28%)	9,12,14	2.75	5 (55%)
2	OZT	T	1	2	7,9,10	2.58	2 (28%)	9,12,14	2.75	3 (33%)
2	OZT	p	301	2	7,9,10	2.98	2 (28%)	9,12,14	3.29	4 (44%)
2	OZT	t	301	2	7,9,10	2.64	2 (28%)	9,12,14	2.06	4 (44%)
2	OZT	h	301	2	7,9,10	2.85	2 (28%)	9,12,14	2.41	4 (44%)
2	OZT	L	1	2	7,9,10	2.59	2 (28%)	9,12,14	3.02	5 (55%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	OZT	N	1	2	7,9,10	2.68	2 (28%)	9,12,14	2.23	5 (55%)
2	OZT	C	1	2	7,9,10	2.97	2 (28%)	9,12,14	2.48	4 (44%)
2	OZT	P	1	2	7,9,10	2.60	2 (28%)	9,12,14	2.50	5 (55%)
2	OZT	R	1	2	7,9,10	3.08	2 (28%)	9,12,14	3.26	4 (44%)
2	OZT	X	1	2	7,9,10	2.82	2 (28%)	9,12,14	2.51	5 (55%)
2	OZT	E	1	2	7,9,10	3.02	2 (28%)	9,12,14	2.93	6 (66%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	OZT	J	1	2	-	0/1/14/16	0/1/1/1
2	OZT	2	1	2	-	1/1/14/16	0/1/1/1
2	OZT	4	301	2	-	1/1/14/16	0/1/1/1
2	OZT	Z	1	2	-	0/1/14/16	0/1/1/1
2	OZT	n	301	2	-	1/1/14/16	0/1/1/1
2	OZT	l	301	2	-	0/1/14/16	0/1/1/1
2	OZT	z	301	2	-	0/1/14/16	0/1/1/1
2	OZT	H	1	2	-	0/1/14/16	0/1/1/1
2	OZT	v	301	2	-	0/1/14/16	0/1/1/1
2	OZT	r	301	2	-	0/1/14/16	0/1/1/1
2	OZT	c	301	2	-	0/1/14/16	0/1/1/1
2	OZT	G	1	2	-	0/1/14/16	0/1/1/1
2	OZT	e	301	2	-	0/1/14/16	0/1/1/1
2	OZT	g	301	2	-	0/1/14/16	0/1/1/1
2	OZT	j	301	2	-	0/1/14/16	0/1/1/1
2	OZT	V	1	2	-	0/1/14/16	0/1/1/1
2	OZT	x	301	2	-	0/1/14/16	0/1/1/1
2	OZT	T	1	2	-	0/1/14/16	0/1/1/1
2	OZT	p	301	2	-	0/1/14/16	0/1/1/1
2	OZT	t	301	2	-	1/1/14/16	0/1/1/1
2	OZT	h	301	2	-	0/1/14/16	0/1/1/1
2	OZT	L	1	2	-	0/1/14/16	0/1/1/1
2	OZT	N	1	2	-	0/1/14/16	0/1/1/1
2	OZT	C	1	2	-	0/1/14/16	0/1/1/1
2	OZT	P	1	2	-	0/1/14/16	0/1/1/1
2	OZT	R	1	2	-	1/1/14/16	0/1/1/1
2	OZT	X	1	2	-	1/1/14/16	0/1/1/1
2	OZT	E	1	2	-	0/1/14/16	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	x	301	OZT	O1-C5	7.55	1.46	1.36
2	z	301	OZT	O1-C5	7.53	1.46	1.36
2	n	301	OZT	O1-C5	7.49	1.46	1.36
2	E	1	OZT	O1-C5	7.34	1.46	1.36
2	4	301	OZT	O1-C5	7.33	1.46	1.36

The worst 5 of 122 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	z	301	OZT	C7-C2-CA	-7.57	104.16	114.80
2	p	301	OZT	C7-C2-CA	-6.88	105.13	114.80
2	T	1	OZT	C7-C2-CA	-6.64	105.46	114.80
2	v	301	OZT	C7-C2-CA	-6.57	105.56	114.80
2	Z	1	OZT	C7-C2-CA	-6.32	105.92	114.80

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	t	301	OZT	O-C-CA-C2
2	R	1	OZT	O-C-CA-C2
2	2	1	OZT	O-C-CA-C2
2	4	301	OZT	O-C-CA-C2
2	n	301	OZT	O-C-CA-C2

There are no ring outliers.

12 monomers are involved in 43 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	J	1	OZT	1	0
2	2	1	OZT	6	0
2	4	301	OZT	5	0
2	Z	1	OZT	1	0
2	H	1	OZT	8	0
2	V	1	OZT	2	0
2	L	1	OZT	4	0
2	N	1	OZT	2	0
2	C	1	OZT	2	0
2	P	1	OZT	2	0
2	X	1	OZT	6	0
2	E	1	OZT	4	0

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS failed to run properly - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

EDS failed to run properly - this section is therefore empty.

6.3 Carbohydrates ⓘ

EDS failed to run properly - this section is therefore empty.

6.4 Ligands ⓘ

EDS failed to run properly - this section is therefore empty.

6.5 Other polymers ⓘ

EDS failed to run properly - this section is therefore empty.