



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 09:11 AM GMT

PDB ID : 3H6F
Title : Crystal Structure of Mycobacterium Tuberculosis Proteasome Modified by inhibitor HT1171
Authors : Li, D.; Li, H.; Lin, G.
Deposited on : 2009-04-23
Resolution : 2.51 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

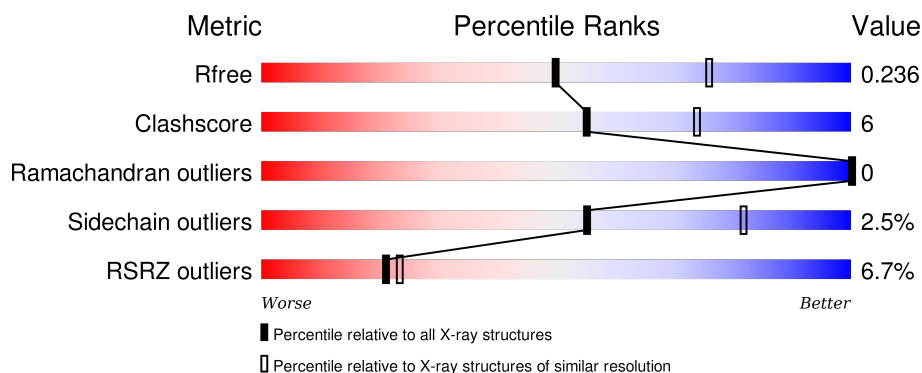
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.51 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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>77%</div> <div>8%</div> <div>13%</div> </div>
1	A	248	<div> <div>10%</div> <div>76%</div> <div>10%</div> <div>13%</div> </div>
1	B	248	<div> <div>7%</div> <div>78%</div> <div>8%</div> <div>14%</div> </div>
1	D	248	<div> <div>11%</div> <div>75%</div> <div>10%</div> <div>14%</div> </div>
1	F	248	<div> <div>6%</div> <div>78%</div> <div>8%</div> <div>13%</div> </div>

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Mol	Chain	Length	Quality of chain
1	I	248	
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
3	DMF	1	250	-	-	-	X
3	DMF	2	42	-	-	-	X
3	DMF	2	49	-	-	-	X
3	DMF	2	52	-	-	-	X
3	DMF	B	250	-	-	-	X
3	DMF	C	10	-	-	-	X
3	DMF	C	47	-	-	-	X
3	DMF	C	55	-	-	X	X
3	DMF	D	249	-	-	-	X
3	DMF	E	20	-	-	-	X
3	DMF	E	28	-	-	-	X
3	DMF	E	66	-	-	-	X
3	DMF	G	1	-	-	-	X
3	DMF	G	12	-	-	-	X
3	DMF	G	24	-	-	-	X
3	DMF	G	60	-	-	-	X
3	DMF	G	64	-	-	-	X
3	DMF	H	26	-	-	-	X
3	DMF	H	32	-	-	-	X
3	DMF	I	249	-	-	-	X
3	DMF	J	4	-	-	X	X
3	DMF	J	45	-	-	-	X
3	DMF	J	50	-	-	-	X
3	DMF	K	250	-	-	-	X
3	DMF	K	251	-	-	-	X
3	DMF	L	3	-	-	-	X
3	DMF	L	36	-	-	-	X
3	DMF	L	53	-	-	-	X
3	DMF	M	249	-	-	-	X
3	DMF	M	250	-	-	-	X
3	DMF	N	15	-	-	-	X
3	DMF	N	22	-	-	-	X
3	DMF	N	58	-	-	-	X
3	DMF	O	249	-	-	-	X
3	DMF	P	14	-	-	-	X
3	DMF	P	51	-	-	-	X
3	DMF	P	56	-	-	-	X
3	DMF	R	34	-	-	-	X
3	DMF	R	59	-	-	-	X
3	DMF	S	249	-	-	-	X
3	DMF	T	29	-	-	X	X
3	DMF	T	67	-	-	-	X
3	DMF	U	249	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	DMF	V	27	-	-	-	X
3	DMF	W	249	-	-	-	X
3	DMF	X	16	-	-	-	X
3	DMF	X	61	-	-	-	X
3	DMF	Z	18	-	-	-	X
3	DMF	Z	30	-	-	-	X
3	DMF	Z	54	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 47697 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Proteasome (Alpha subunit) PrcA.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	215	Total 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	222	Total 1638	C 1025	N 281	O 328	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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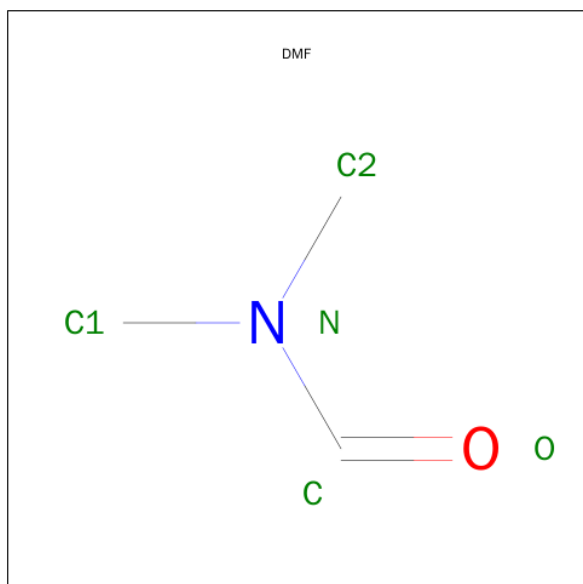
Chain	Residue	Modelled	Actual	Comment	Reference
P	539	HIS	-	EXPRESSION TAG	UNP O33245
P	540	HIS	-	EXPRESSION TAG	UNP O33245
R	301	OZT	-	INSERTION	UNP O33245
R	535	HIS	-	EXPRESSION TAG	UNP O33245
R	536	HIS	-	EXPRESSION TAG	UNP O33245
R	537	HIS	-	EXPRESSION TAG	UNP O33245
R	538	HIS	-	EXPRESSION TAG	UNP 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	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	D	1	Total	C	N	O	0	0
			5	3	1	1		
3	E	1	Total	C	N	O	0	0
			5	3	1	1		
3	E	1	Total	C	N	O	0	0
			5	3	1	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	E	1	Total 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	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
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	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

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
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
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	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	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	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

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	W	1	Total	C	N	O	0	0
			5	3	1	1		
3	X	1	Total	C	N	O	0	0
			5	3	1	1		
3	X	1	Total	C	N	O	0	0
			5	3	1	1		
3	X	1	Total	C	N	O	0	0
			5	3	1	1		
3	Z	1	Total	C	N	O	0	0
			5	3	1	1		
3	Z	1	Total	C	N	O	0	0
			5	3	1	1		
3	Z	1	Total	C	N	O	0	0
			5	3	1	1		
3	Z	1	Total	C	N	O	0	0
			5	3	1	1		
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		
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	34	Total	O	0	0
			34	34		
4	B	40	Total	O	0	0
			40	40		
4	C	95	Total	O	0	0
			95	95		
4	D	49	Total	O	0	0
			49	49		

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

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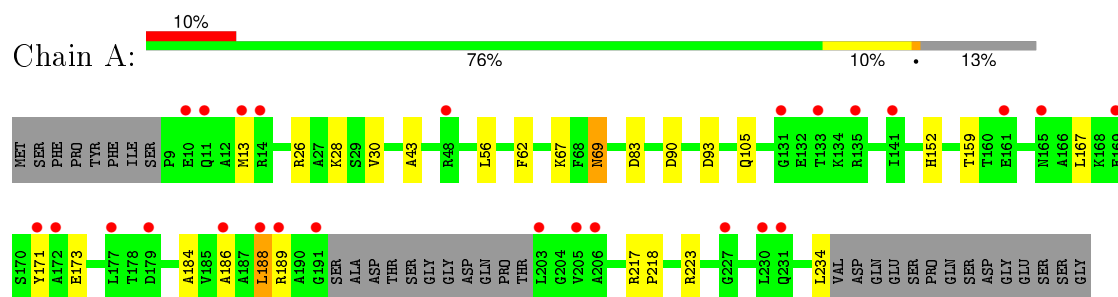
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	Z	85	Total 85	O 85	0	0
4	1	34	Total 34	O 34	0	0
4	2	93	Total 93	O 93	0	0

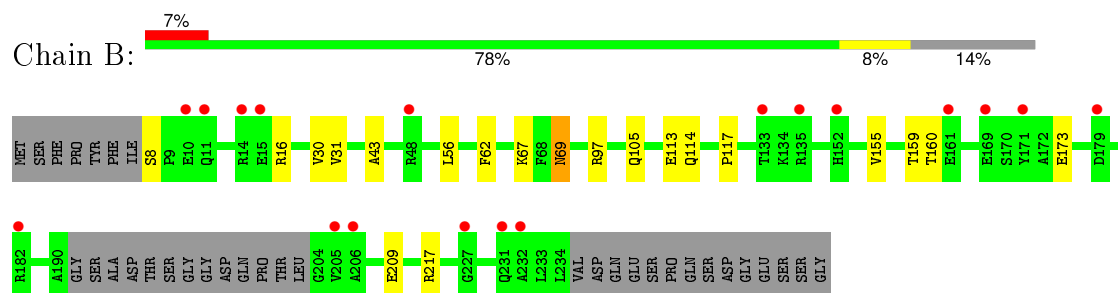
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

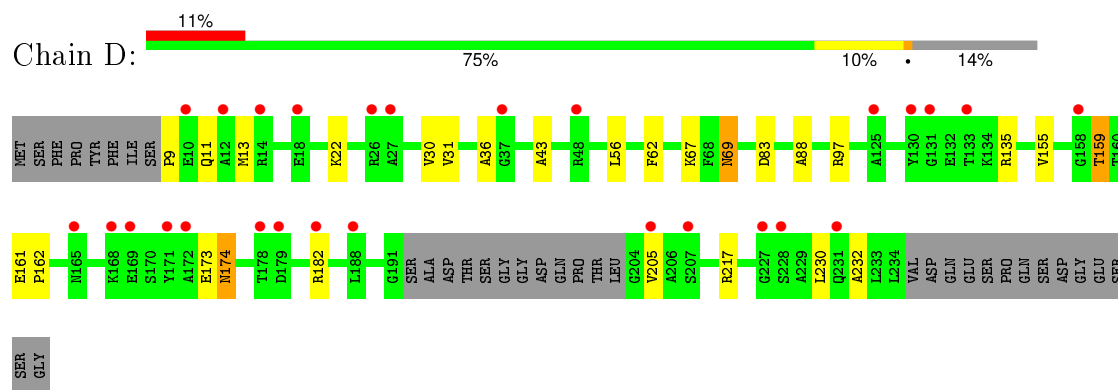
• Molecule 1: Proteasome (Alpha subunit) PrcA



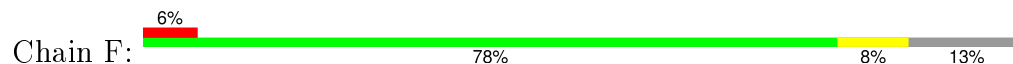
• Molecule 1: Proteasome (Alpha subunit) PrcA

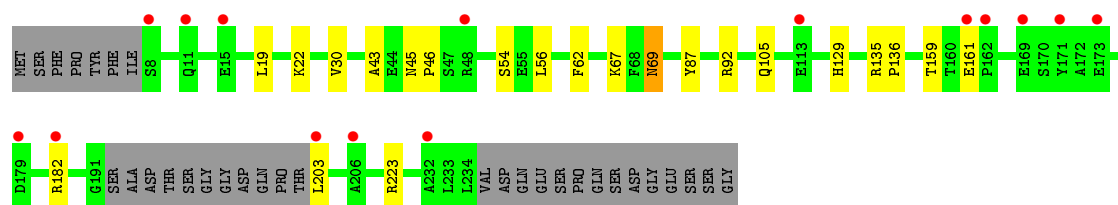


• Molecule 1: Proteasome (Alpha subunit) PrcA



• Molecule 1: Proteasome (Alpha subunit) PrcA

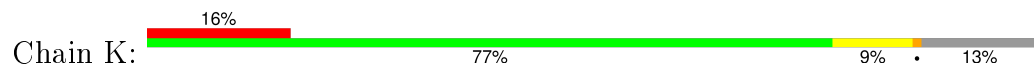




• Molecule 1: Proteasome (Alpha subunit) PrcA



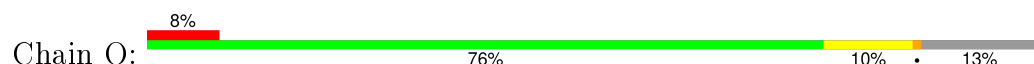
• Molecule 1: Proteasome (Alpha subunit) PrcA

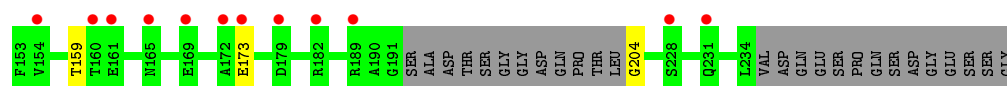


• Molecule 1: Proteasome (Alpha subunit) PrcA

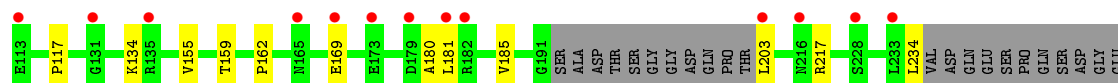
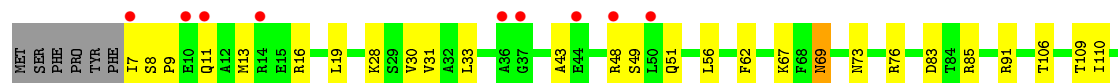


• Molecule 1: Proteasome (Alpha subunit) PrcA

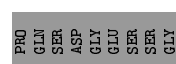
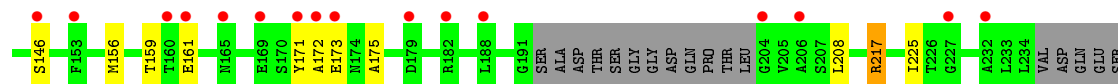
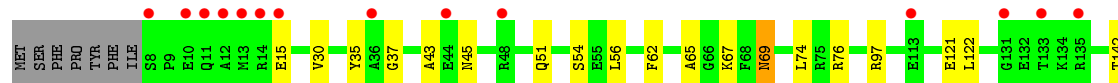




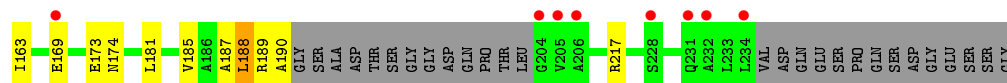
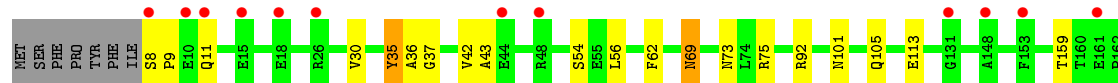
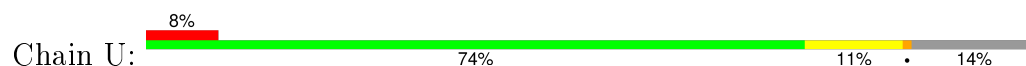
• Molecule 1: Proteasome (Alpha subunit) PrcA



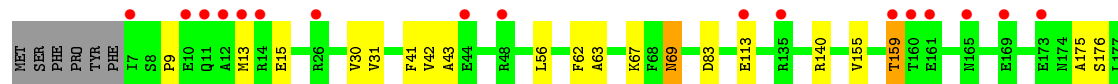
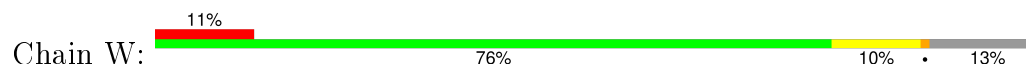
• Molecule 1: Proteasome (Alpha subunit) PrcA



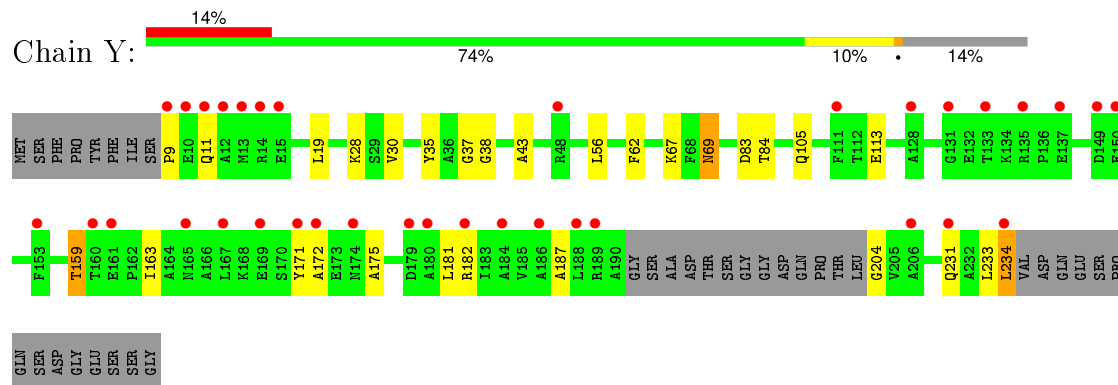
• Molecule 1: Proteasome (Alpha subunit) PrcA



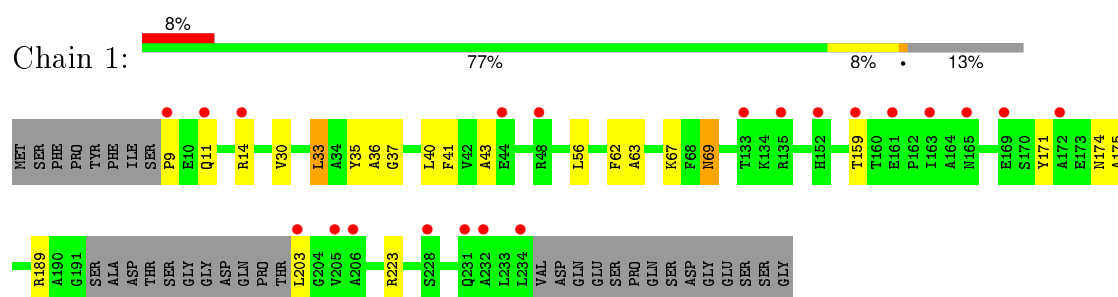
• Molecule 1: Proteasome (Alpha subunit) PrcA



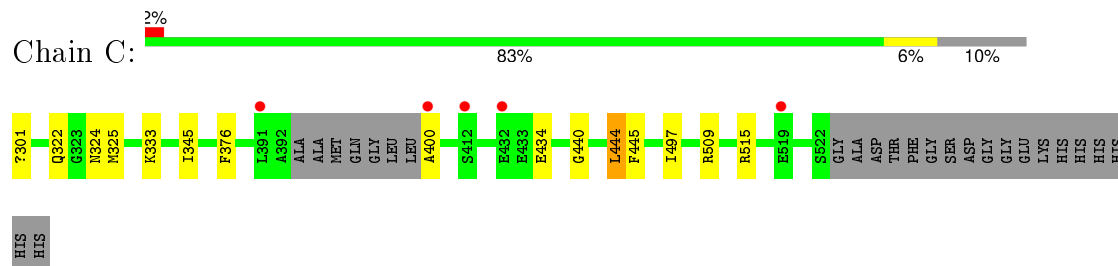
- Molecule 1: Proteasome (Alpha subunit) PrcA



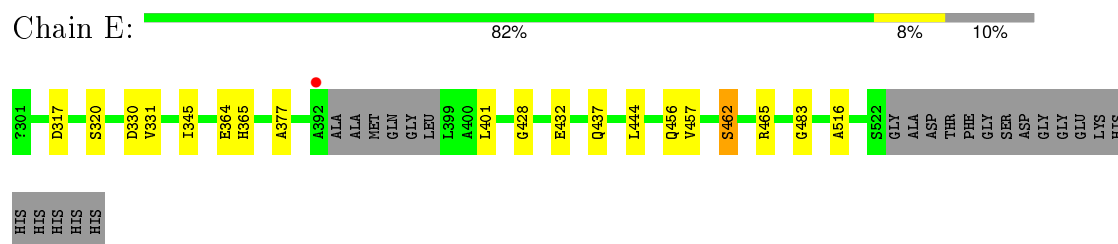
- Molecule 1: Proteasome (Alpha subunit) PrcA



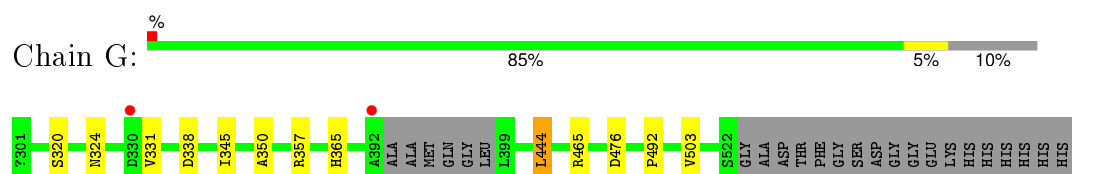
- Molecule 2: Proteasome (Beta subunit) PrcB



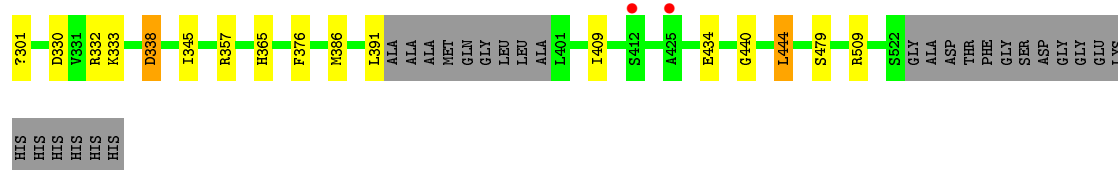
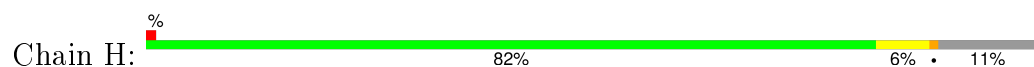
- Molecule 2: Proteasome (Beta subunit) PrcB



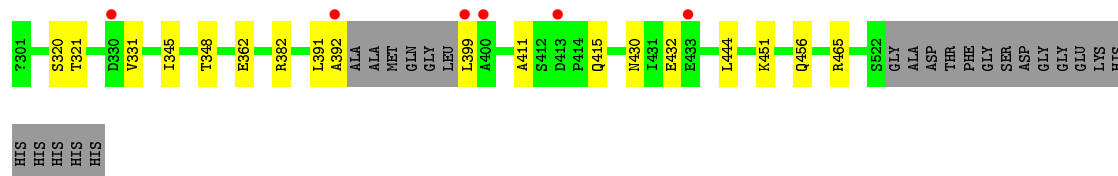
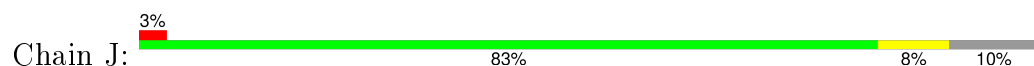
- Molecule 2: Proteasome (Beta subunit) PrcB



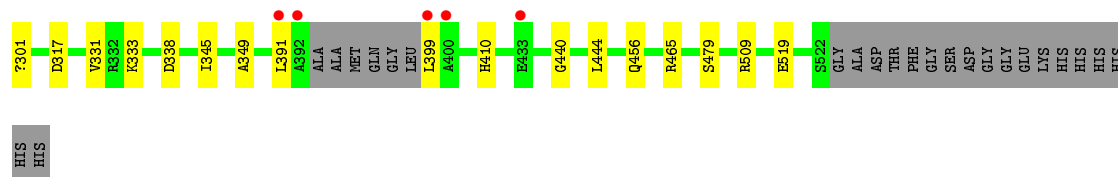
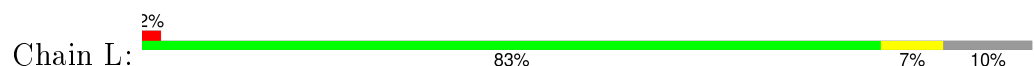
- Molecule 2: Proteasome (Beta subunit) PrcB



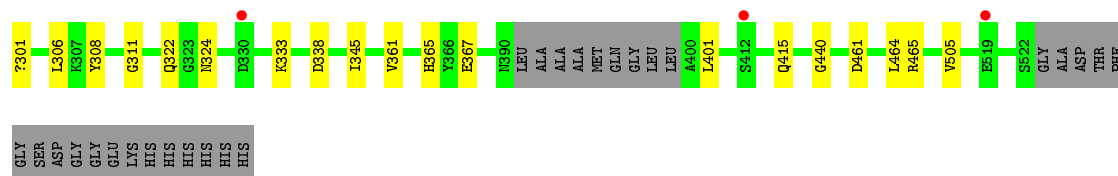
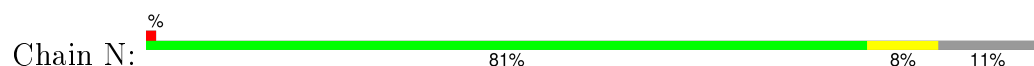
- Molecule 2: Proteasome (Beta subunit) PrcB

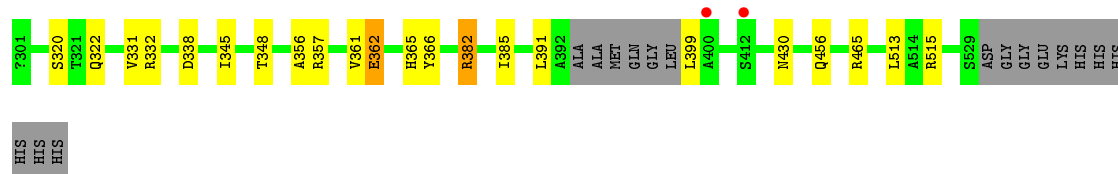


- Molecule 2: Proteasome (Beta subunit) PrcB

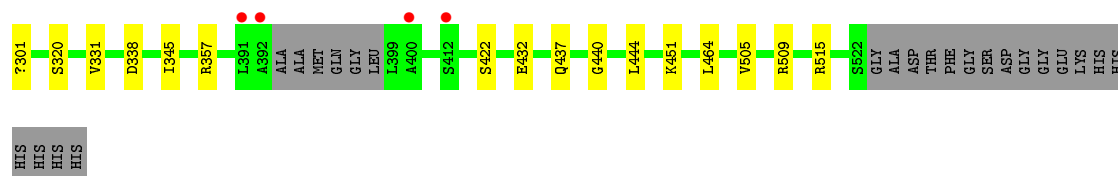
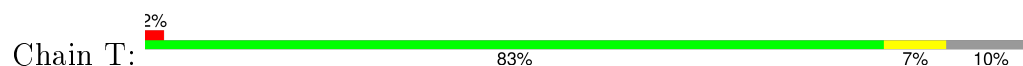


- Molecule 2: Proteasome (Beta subunit) PrcB

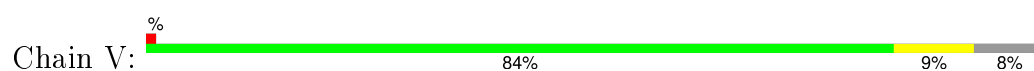




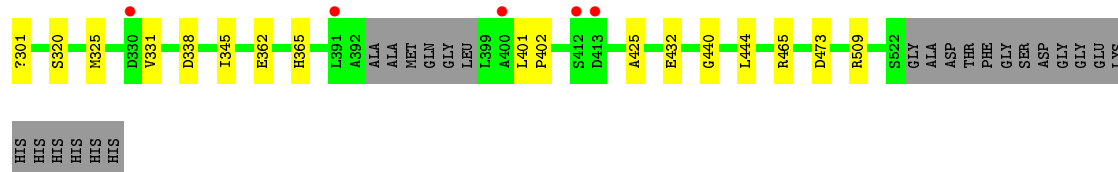
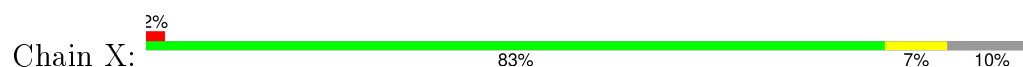
• Molecule 2: Proteasome (Beta subunit) PrcB



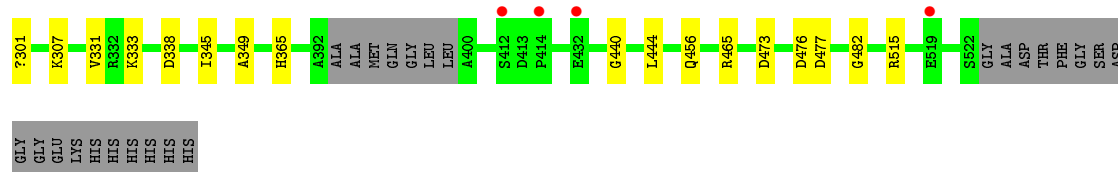
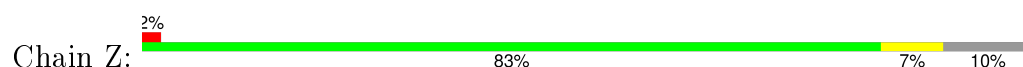
• Molecule 2: Proteasome (Beta subunit) PrcB



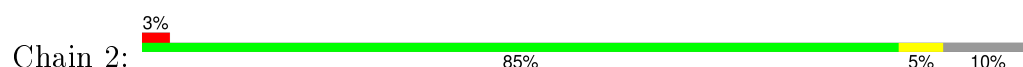
• Molecule 2: Proteasome (Beta subunit) PrcB



• 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, α , β , γ	171.98Å 118.04Å 197.06Å 90.00° 113.62° 90.00°	Depositor
Resolution (Å)	29.83 – 2.51 33.75 – 2.51	Depositor EDS
% Data completeness (in resolution range)	94.2 (29.83-2.51) 94.4 (33.75-2.51)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.84 (at 2.51Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.216 , 0.238 0.216 , 0.236	Depositor DCC
R_{free} test set	11629 reflections (4.99%)	DCC
Wilson B-factor (Å ²)	27.5	Xtriage
Anisotropy	0.239	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 42.2	EDS
Estimated twinning fraction	0.004 for h,-k,-h-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	4 of 235343 reflections (0.002%)	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	47697	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

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

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	0.68	0/1681	0.78	0/2270
1	A	0.71	0/1681	0.76	0/2270
1	B	0.67	0/1675	0.77	0/2263
1	D	0.69	0/1673	0.78	0/2259
1	F	0.68	0/1687	0.76	0/2279
1	I	0.72	1/1677 (0.1%)	0.79	0/2265
1	K	0.68	0/1681	0.77	0/2270
1	M	0.71	0/1683	0.80	2/2274 (0.1%)
1	O	0.75	0/1679	0.78	0/2268
1	Q	0.67	0/1695	0.77	0/2290
1	S	0.66	0/1679	0.78	1/2268 (0.0%)
1	U	0.76	0/1675	0.79	0/2263
1	W	0.66	0/1695	0.77	0/2290
1	Y	0.66	0/1669	0.77	0/2254
2	2	0.71	0/1607	0.76	0/2178
2	C	0.76	0/1607	0.77	0/2178
2	E	0.81	1/1615 (0.1%)	0.79	0/2189
2	G	0.68	0/1615	0.75	0/2189
2	H	0.72	0/1597	0.76	1/2164 (0.0%)
2	J	0.75	0/1615	0.78	0/2189
2	L	0.77	0/1615	0.77	0/2189
2	N	0.76	0/1594	0.77	0/2160
2	P	0.74	0/1615	0.76	0/2189
2	R	0.79	1/1661 (0.1%)	0.76	0/2251
2	T	0.78	0/1615	0.78	1/2189 (0.0%)
2	V	0.78	0/1653	0.76	0/2240
2	X	0.72	0/1615	0.76	0/2189
2	Z	0.75	0/1607	0.76	0/2178
All	All	0.72	3/46161 (0.0%)	0.77	5/62455 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	516	ALA	CA-CB	-5.67	1.40	1.52
2	R	366	TYR	CD1-CE1	-5.25	1.31	1.39
1	I	172	ALA	CA-CB	-5.09	1.41	1.52

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	90	ASP	CB-CG-OD1	5.58	123.32	118.30
1	M	234	LEU	CA-CB-CG	5.51	127.97	115.30
2	H	338	ASP	CB-CG-OD1	5.22	123.00	118.30
1	S	208	LEU	CA-CB-CG	5.12	127.08	115.30
2	T	338	ASP	CB-CG-OD1	5.01	122.81	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	1656	0	1658	24	0
1	A	1656	0	1658	22	0
1	B	1650	0	1648	21	0
1	D	1648	0	1647	37	0
1	F	1662	0	1662	22	0
1	I	1652	0	1655	19	0
1	K	1656	0	1658	29	0
1	M	1658	0	1659	40	0
1	O	1654	0	1651	29	0
1	Q	1670	0	1673	40	0
1	S	1654	0	1651	28	0
1	U	1650	0	1648	25	0
1	W	1670	0	1673	24	0
1	Y	1644	0	1644	37	0
2	2	1593	0	1577	11	0
2	C	1593	0	1577	15	0
2	E	1601	0	1588	15	0
2	G	1601	0	1588	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	H	1583	0	1567	15	0
2	J	1601	0	1588	17	0
2	L	1601	0	1588	9	0
2	N	1580	0	1561	13	0
2	P	1601	0	1588	11	0
2	R	1646	0	1624	20	0
2	T	1601	0	1588	11	0
2	V	1638	0	1613	20	0
2	X	1601	0	1588	15	0
2	Z	1593	0	1577	14	0
3	1	10	0	14	0	0
3	2	20	0	28	0	0
3	A	5	0	7	0	0
3	B	10	0	14	0	0
3	C	20	0	28	6	0
3	D	5	0	7	0	0
3	E	15	0	21	3	0
3	F	5	0	7	0	0
3	G	25	0	35	2	0
3	H	20	0	28	0	0
3	I	10	0	14	0	0
3	J	15	0	21	5	0
3	K	15	0	21	1	0
3	L	15	0	21	2	0
3	M	10	0	14	2	0
3	N	20	0	28	1	0
3	O	5	0	7	0	0
3	P	20	0	28	1	0
3	Q	5	0	7	0	0
3	R	10	0	14	2	0
3	S	5	0	7	0	0
3	T	10	0	14	4	0
3	U	5	0	7	0	0
3	V	10	0	14	1	0
3	W	5	0	7	0	0
3	X	15	0	21	1	0
3	Z	25	0	35	2	0
4	1	34	0	0	9	0
4	2	93	0	0	4	0
4	A	34	0	0	8	0
4	B	40	0	0	13	0
4	C	95	0	0	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	49	0	0	10	0
4	E	89	0	0	5	0
4	F	40	0	0	15	0
4	G	72	0	0	4	0
4	H	91	0	0	11	0
4	I	38	0	0	10	0
4	J	90	0	0	13	0
4	K	39	0	0	17	0
4	L	90	0	0	4	0
4	M	42	0	0	22	0
4	N	86	0	0	4	0
4	O	40	0	0	17	0
4	P	82	0	0	4	0
4	Q	34	0	0	14	0
4	R	97	0	0	5	0
4	S	34	0	0	17	0
4	T	78	0	0	9	0
4	U	38	0	0	7	0
4	V	104	0	0	4	0
4	W	27	0	0	11	0
4	X	84	0	0	10	0
4	Y	24	0	0	14	0
4	Z	85	0	0	7	0
All	All	47697	0	45866	582	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 6.

The worst 5 of 582 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:173:GLU:C	1:D:174:ASN:HD22	1.40	1.24
2:J:432:GLU:HG2	4:J:1761:HOH:O	1.37	1.21
1:I:140:ARG:HD2	4:I:1512:HOH:O	1.41	1.19
2:P:399:LEU:HD12	4:P:1556:HOH:O	1.36	1.19
2:E:432:GLU:HG2	4:E:1322:HOH:O	1.42	1.18

There are no symmetry-related clashes.

5.3 Torsion angles

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

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

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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%)	161 (98%)	3 (2%)	66	88
1	A	164/192 (85%)	159 (97%)	5 (3%)	48	76
1	B	164/192 (85%)	161 (98%)	3 (2%)	66	88
1	D	163/192 (85%)	160 (98%)	3 (2%)	66	88
1	F	165/192 (86%)	163 (99%)	2 (1%)	78	93
1	I	164/192 (85%)	158 (96%)	6 (4%)	41	68
1	K	164/192 (85%)	159 (97%)	5 (3%)	48	76
1	M	165/192 (86%)	161 (98%)	4 (2%)	57	82
1	O	164/192 (85%)	159 (97%)	5 (3%)	48	76
1	Q	166/192 (86%)	160 (96%)	6 (4%)	42	69
1	S	164/192 (85%)	161 (98%)	3 (2%)	66	88
1	U	164/192 (85%)	156 (95%)	8 (5%)	31	55
1	W	166/192 (86%)	161 (97%)	5 (3%)	48	76
1	Y	163/192 (85%)	159 (98%)	4 (2%)	55	82
2	2	160/177 (90%)	157 (98%)	3 (2%)	65	87
2	C	160/177 (90%)	155 (97%)	5 (3%)	47	75
2	E	161/177 (91%)	156 (97%)	5 (3%)	47	75
2	G	161/177 (91%)	156 (97%)	5 (3%)	47	75

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	H	160/177 (90%)	154 (96%)	6 (4%)	40	67
2	J	161/177 (91%)	160 (99%)	1 (1%)	90	97
2	L	161/177 (91%)	157 (98%)	4 (2%)	55	82
2	N	159/177 (90%)	154 (97%)	5 (3%)	47	75
2	P	161/177 (91%)	158 (98%)	3 (2%)	65	87
2	R	165/177 (93%)	159 (96%)	6 (4%)	42	69
2	T	161/177 (91%)	159 (99%)	2 (1%)	78	93
2	V	164/177 (93%)	161 (98%)	3 (2%)	66	88
2	X	161/177 (91%)	159 (99%)	2 (1%)	78	93
2	Z	160/177 (90%)	157 (98%)	3 (2%)	65	87
All	All	4555/5166 (88%)	4440 (98%)	115 (2%)	55	82

5 of 115 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	M	181	LEU
2	P	322	GLN
2	Z	338	ASP
1	M	188	LEU
2	N	465	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 66 such sidechains are listed below:

Mol	Chain	Res	Type
1	M	51	GLN
1	O	98	GLN
2	Z	365	HIS
1	M	69	ASN
2	N	456	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	2	301	2	8,9,10	3.65	4 (50%)	7,12,14	4.58	5 (71%)
2	OZT	C	301	2	8,9,10	4.05	4 (50%)	7,12,14	4.51	5 (71%)
2	OZT	E	301	2	8,9,10	4.11	4 (50%)	7,12,14	4.28	5 (71%)
2	OZT	G	301	2	8,9,10	3.77	3 (37%)	7,12,14	4.51	5 (71%)
2	OZT	H	301	2	8,9,10	3.88	4 (50%)	7,12,14	4.65	4 (57%)
2	OZT	J	301	2	8,9,10	3.91	4 (50%)	7,12,14	4.70	5 (71%)
2	OZT	L	301	2	8,9,10	4.02	4 (50%)	7,12,14	4.65	5 (71%)
2	OZT	N	301	2	8,9,10	3.74	4 (50%)	7,12,14	4.61	5 (71%)
2	OZT	P	301	2	8,9,10	3.74	4 (50%)	7,12,14	4.61	5 (71%)
2	OZT	R	301	2	8,9,10	4.10	4 (50%)	7,12,14	4.33	5 (71%)
2	OZT	T	301	2	8,9,10	3.79	4 (50%)	7,12,14	4.73	5 (71%)
2	OZT	V	301	2	8,9,10	3.86	4 (50%)	7,12,14	4.71	5 (71%)
2	OZT	X	301	2	8,9,10	3.83	4 (50%)	7,12,14	4.50	4 (57%)
2	OZT	Z	301	2	8,9,10	3.83	4 (50%)	7,12,14	4.49	4 (57%)

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	2	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	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	H	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	L	301	2	-	0/1/14/16	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	OZT	N	301	2	-	0/1/14/16	0/1/1/1
2	OZT	P	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	T	301	2	-	0/1/14/16	0/1/1/1
2	OZT	V	301	2	-	0/1/14/16	0/1/1/1
2	OZT	X	301	2	-	0/1/14/16	0/1/1/1
2	OZT	Z	301	2	-	0/1/14/16	0/1/1/1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	X	301	OZT	C2-CA	-3.99	1.45	1.54
2	H	301	OZT	C2-CA	-3.66	1.46	1.54
2	Z	301	OZT	C2-CA	-3.55	1.46	1.54
2	R	301	OZT	C2-CA	-3.36	1.47	1.54
2	P	301	OZT	C2-CA	-3.36	1.47	1.54

The worst 5 of 67 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	301	OZT	O6-C5-N	-7.25	120.35	129.16
2	H	301	OZT	O6-C5-N	-7.13	120.50	129.16
2	T	301	OZT	O6-C5-N	-7.04	120.61	129.16
2	X	301	OZT	O6-C5-N	-7.04	120.61	129.16
2	L	301	OZT	O6-C5-N	-6.99	120.67	129.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

9 monomers are involved in 15 short contacts:

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

67 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	DMF	1	249	-	4,4,4	0.54	0	4,4,4	0.29	0
3	DMF	1	250	-	4,4,4	0.55	0	4,4,4	0.28	0
3	DMF	2	42	-	4,4,4	0.34	0	4,4,4	0.31	0
3	DMF	2	49	-	4,4,4	0.49	0	4,4,4	0.34	0
3	DMF	2	52	-	4,4,4	0.50	0	4,4,4	0.29	0
3	DMF	2	63	-	4,4,4	0.56	0	4,4,4	0.36	0
3	DMF	A	249	-	4,4,4	0.46	0	4,4,4	0.28	0
3	DMF	B	249	-	4,4,4	0.59	0	4,4,4	0.27	0
3	DMF	B	250	-	4,4,4	0.54	0	4,4,4	0.30	0
3	DMF	C	10	-	4,4,4	0.45	0	4,4,4	0.39	0
3	DMF	C	38	-	4,4,4	0.25	0	4,4,4	0.32	0
3	DMF	C	47	-	4,4,4	0.50	0	4,4,4	0.36	0
3	DMF	C	55	-	4,4,4	0.28	0	4,4,4	0.55	0
3	DMF	D	249	-	4,4,4	0.47	0	4,4,4	0.35	0
3	DMF	E	20	-	4,4,4	0.53	0	4,4,4	0.32	0
3	DMF	E	28	-	4,4,4	0.56	0	4,4,4	0.28	0
3	DMF	E	66	-	4,4,4	0.62	0	4,4,4	0.30	0
3	DMF	F	249	-	4,4,4	0.52	0	4,4,4	0.29	0
3	DMF	G	1	-	4,4,4	0.38	0	4,4,4	0.40	0
3	DMF	G	12	-	4,4,4	0.49	0	4,4,4	0.27	0
3	DMF	G	24	-	4,4,4	0.49	0	4,4,4	0.28	0
3	DMF	G	60	-	4,4,4	0.51	0	4,4,4	0.34	0
3	DMF	G	64	-	4,4,4	0.53	0	4,4,4	0.38	0
3	DMF	H	26	-	4,4,4	0.55	0	4,4,4	0.29	0
3	DMF	H	32	-	4,4,4	0.63	0	4,4,4	0.34	0
3	DMF	H	33	-	4,4,4	0.58	0	4,4,4	0.35	0
3	DMF	H	62	-	4,4,4	0.65	0	4,4,4	0.33	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	DMF	I	249	-	4,4,4	0.62	0	4,4,4	0.27	0
3	DMF	I	250	-	4,4,4	0.52	0	4,4,4	0.28	0
3	DMF	J	4	-	4,4,4	0.50	0	4,4,4	0.33	0
3	DMF	J	45	-	4,4,4	0.55	0	4,4,4	0.35	0
3	DMF	J	50	-	4,4,4	0.45	0	4,4,4	0.30	0
3	DMF	K	249	-	4,4,4	0.51	0	4,4,4	0.28	0
3	DMF	K	250	-	4,4,4	0.56	0	4,4,4	0.37	0
3	DMF	K	251	-	4,4,4	0.44	0	4,4,4	0.29	0
3	DMF	L	3	-	4,4,4	0.29	0	4,4,4	0.30	0
3	DMF	L	36	-	4,4,4	0.43	0	4,4,4	0.36	0
3	DMF	L	53	-	4,4,4	0.46	0	4,4,4	0.36	0
3	DMF	M	249	-	4,4,4	0.48	0	4,4,4	0.32	0
3	DMF	M	250	-	4,4,4	0.69	0	4,4,4	0.35	0
3	DMF	N	15	-	4,4,4	0.44	0	4,4,4	0.27	0
3	DMF	N	2	-	4,4,4	0.51	0	4,4,4	0.26	0
3	DMF	N	22	-	4,4,4	0.53	0	4,4,4	0.31	0
3	DMF	N	58	-	4,4,4	0.47	0	4,4,4	0.35	0
3	DMF	O	249	-	4,4,4	0.41	0	4,4,4	0.33	0
3	DMF	P	14	-	4,4,4	0.47	0	4,4,4	0.29	0
3	DMF	P	51	-	4,4,4	0.64	0	4,4,4	0.30	0
3	DMF	P	56	-	4,4,4	0.45	0	4,4,4	0.29	0
3	DMF	P	65	-	4,4,4	0.58	0	4,4,4	0.31	0
3	DMF	Q	249	-	4,4,4	0.60	0	4,4,4	0.28	0
3	DMF	R	34	-	4,4,4	0.17	0	4,4,4	0.43	0
3	DMF	R	59	-	4,4,4	0.58	0	4,4,4	0.34	0
3	DMF	S	249	-	4,4,4	0.50	0	4,4,4	0.27	0
3	DMF	T	29	-	4,4,4	0.51	0	4,4,4	0.30	0
3	DMF	T	67	-	4,4,4	0.52	0	4,4,4	1.18	0
3	DMF	U	249	-	4,4,4	0.42	0	4,4,4	0.28	0
3	DMF	V	27	-	4,4,4	0.23	0	4,4,4	0.45	0
3	DMF	V	39	-	4,4,4	0.56	0	4,4,4	0.31	0
3	DMF	W	249	-	4,4,4	0.47	0	4,4,4	0.30	0
3	DMF	X	16	-	4,4,4	0.49	0	4,4,4	0.32	0
3	DMF	X	40	-	4,4,4	0.59	0	4,4,4	0.30	0
3	DMF	X	61	-	4,4,4	0.40	0	4,4,4	0.36	0
3	DMF	Z	18	-	4,4,4	0.42	0	4,4,4	0.34	0
3	DMF	Z	30	-	4,4,4	0.39	0	4,4,4	0.33	0
3	DMF	Z	41	-	4,4,4	0.49	0	4,4,4	0.31	0
3	DMF	Z	43	-	4,4,4	0.58	0	4,4,4	0.28	0
3	DMF	Z	54	-	4,4,4	0.51	0	4,4,4	0.31	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	1	249	-	-	0/2/2/2	0/0/0/0
3	DMF	1	250	-	-	0/2/2/2	0/0/0/0
3	DMF	2	42	-	-	0/2/2/2	0/0/0/0
3	DMF	2	49	-	-	0/2/2/2	0/0/0/0
3	DMF	2	52	-	-	0/2/2/2	0/0/0/0
3	DMF	2	63	-	-	0/2/2/2	0/0/0/0
3	DMF	A	249	-	-	0/2/2/2	0/0/0/0
3	DMF	B	249	-	-	0/2/2/2	0/0/0/0
3	DMF	B	250	-	-	0/2/2/2	0/0/0/0
3	DMF	C	10	-	-	0/2/2/2	0/0/0/0
3	DMF	C	38	-	-	0/2/2/2	0/0/0/0
3	DMF	C	47	-	-	0/2/2/2	0/0/0/0
3	DMF	C	55	-	-	0/2/2/2	0/0/0/0
3	DMF	D	249	-	-	0/2/2/2	0/0/0/0
3	DMF	E	20	-	-	0/2/2/2	0/0/0/0
3	DMF	E	28	-	-	0/2/2/2	0/0/0/0
3	DMF	E	66	-	-	0/2/2/2	0/0/0/0
3	DMF	F	249	-	-	0/2/2/2	0/0/0/0
3	DMF	G	1	-	-	0/2/2/2	0/0/0/0
3	DMF	G	12	-	-	0/2/2/2	0/0/0/0
3	DMF	G	24	-	-	0/2/2/2	0/0/0/0
3	DMF	G	60	-	-	0/2/2/2	0/0/0/0
3	DMF	G	64	-	-	0/2/2/2	0/0/0/0
3	DMF	H	26	-	-	0/2/2/2	0/0/0/0
3	DMF	H	32	-	-	0/2/2/2	0/0/0/0
3	DMF	H	33	-	-	0/2/2/2	0/0/0/0
3	DMF	H	62	-	-	0/2/2/2	0/0/0/0
3	DMF	I	249	-	-	0/2/2/2	0/0/0/0
3	DMF	I	250	-	-	0/2/2/2	0/0/0/0
3	DMF	J	4	-	-	0/2/2/2	0/0/0/0
3	DMF	J	45	-	-	0/2/2/2	0/0/0/0
3	DMF	J	50	-	-	0/2/2/2	0/0/0/0
3	DMF	K	249	-	-	0/2/2/2	0/0/0/0
3	DMF	K	250	-	-	0/2/2/2	0/0/0/0
3	DMF	K	251	-	-	0/2/2/2	0/0/0/0
3	DMF	L	3	-	-	0/2/2/2	0/0/0/0
3	DMF	L	36	-	-	0/2/2/2	0/0/0/0
3	DMF	L	53	-	-	0/2/2/2	0/0/0/0
3	DMF	M	249	-	-	0/2/2/2	0/0/0/0
3	DMF	M	250	-	-	0/2/2/2	0/0/0/0
3	DMF	N	15	-	-	0/2/2/2	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	DMF	N	2	-	-	0/2/2/2	0/0/0/0
3	DMF	N	22	-	-	0/2/2/2	0/0/0/0
3	DMF	N	58	-	-	0/2/2/2	0/0/0/0
3	DMF	O	249	-	-	0/2/2/2	0/0/0/0
3	DMF	P	14	-	-	0/2/2/2	0/0/0/0
3	DMF	P	51	-	-	0/2/2/2	0/0/0/0
3	DMF	P	56	-	-	0/2/2/2	0/0/0/0
3	DMF	P	65	-	-	0/2/2/2	0/0/0/0
3	DMF	Q	249	-	-	0/2/2/2	0/0/0/0
3	DMF	R	34	-	-	0/2/2/2	0/0/0/0
3	DMF	R	59	-	-	0/2/2/2	0/0/0/0
3	DMF	S	249	-	-	0/2/2/2	0/0/0/0
3	DMF	T	29	-	-	0/2/2/2	0/0/0/0
3	DMF	T	67	-	-	0/2/2/2	0/0/0/0
3	DMF	U	249	-	-	0/2/2/2	0/0/0/0
3	DMF	V	27	-	-	0/2/2/2	0/0/0/0
3	DMF	V	39	-	-	0/2/2/2	0/0/0/0
3	DMF	W	249	-	-	0/2/2/2	0/0/0/0
3	DMF	X	16	-	-	0/2/2/2	0/0/0/0
3	DMF	X	40	-	-	0/2/2/2	0/0/0/0
3	DMF	X	61	-	-	0/2/2/2	0/0/0/0
3	DMF	Z	18	-	-	0/2/2/2	0/0/0/0
3	DMF	Z	30	-	-	0/2/2/2	0/0/0/0
3	DMF	Z	41	-	-	0/2/2/2	0/0/0/0
3	DMF	Z	43	-	-	0/2/2/2	0/0/0/0
3	DMF	Z	54	-	-	0/2/2/2	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

15 monomers are involved in 33 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	10	DMF	1	0
3	C	55	DMF	5	0
3	E	66	DMF	3	0
3	G	12	DMF	2	0
3	J	4	DMF	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	K	250	DMF	1	0
3	L	53	DMF	2	0
3	M	249	DMF	2	0
3	N	22	DMF	1	0
3	P	14	DMF	1	0
3	R	34	DMF	2	0
3	T	29	DMF	4	0
3	V	27	DMF	1	0
3	X	40	DMF	1	0
3	Z	18	DMF	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	1	215/248 (86%)	0.54	21 (9%) 10 10	19, 54, 89, 99	0
1	A	215/248 (86%)	0.77	26 (12%) 6 5	18, 54, 91, 98	0
1	B	214/248 (86%)	0.66	18 (8%) 14 14	19, 55, 89, 97	0
1	D	214/248 (86%)	0.78	27 (12%) 5 5	17, 55, 91, 98	0
1	F	216/248 (87%)	0.47	15 (6%) 20 22	19, 55, 87, 95	0
1	I	214/248 (86%)	0.62	24 (11%) 7 7	18, 54, 88, 94	0
1	K	215/248 (86%)	0.81	39 (18%) 2 2	18, 56, 89, 98	0
1	M	215/248 (86%)	0.77	27 (12%) 5 5	19, 53, 88, 98	0
1	O	215/248 (86%)	0.63	20 (9%) 11 11	19, 53, 89, 94	0
1	Q	217/248 (87%)	0.63	22 (10%) 9 9	18, 53, 87, 95	0
1	S	215/248 (86%)	0.70	30 (13%) 4 3	18, 55, 93, 100	0
1	U	214/248 (86%)	0.60	20 (9%) 11 11	18, 54, 91, 96	0
1	W	217/248 (87%)	0.71	28 (12%) 5 4	20, 55, 92, 97	0
1	Y	213/248 (85%)	0.90	35 (16%) 2 2	20, 56, 94, 105	0
2	2	214/240 (89%)	-0.25	8 (3%) 45 50	4, 20, 45, 67	0
2	C	214/240 (89%)	-0.24	5 (2%) 64 67	6, 21, 48, 73	0
2	E	215/240 (89%)	-0.37	1 (0%) 91 92	6, 20, 47, 72	0
2	G	215/240 (89%)	-0.26	2 (0%) 85 88	8, 22, 48, 74	0
2	H	212/240 (88%)	-0.25	2 (0%) 85 88	8, 21, 44, 64	0
2	J	215/240 (89%)	-0.23	6 (2%) 56 61	7, 20, 48, 64	0
2	L	215/240 (89%)	-0.18	5 (2%) 64 67	5, 21, 48, 71	0
2	N	212/240 (88%)	-0.23	3 (1%) 78 80	4, 21, 44, 64	0
2	P	215/240 (89%)	-0.25	5 (2%) 64 67	6, 22, 49, 72	0
2	R	222/240 (92%)	-0.35	2 (0%) 85 88	7, 20, 48, 67	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
2	T	215/240 (89%)	-0.22	4 (1%) 70 73	8, 22, 49, 77	0
2	V	221/240 (92%)	-0.32	2 (0%) 85 88	3, 20, 44, 69	0
2	X	215/240 (89%)	-0.22	5 (2%) 64 67	8, 22, 49, 75	0
2	Z	214/240 (89%)	-0.28	4 (1%) 70 73	9, 23, 48, 64	0
All	All	6023/6832 (88%)	0.21	406 (6%) 21 23	3, 34, 86, 105	0

The worst 5 of 406 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	M	7	ILE	7.5
1	D	169	GLU	7.2
1	D	48	ARG	7.0
1	B	206	ALA	6.9
1	S	8	SER	6.4

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	OZT	H	301	9/10	0.96	0.10	-	22,24,25,28	0
2	OZT	N	301	9/10	0.97	0.08	-	21,24,27,31	0
2	OZT	L	301	9/10	0.93	0.11	-	19,24,26,27	0
2	OZT	R	301	9/10	0.95	0.10	-	20,23,27,28	0
2	OZT	P	301	9/10	0.97	0.12	-	23,28,30,33	0
2	OZT	E	301	9/10	0.98	0.09	-	20,23,25,27	0
2	OZT	V	301	9/10	0.96	0.11	-	20,22,27,31	0
2	OZT	C	301	9/10	0.96	0.10	-	18,23,26,29	0
2	OZT	T	301	9/10	0.98	0.09	-	22,22,24,25	0
2	OZT	Z	301	9/10	0.97	0.10	-	19,21,23,24	0
2	OZT	G	301	9/10	0.95	0.12	-	21,24,29,32	0
2	OZT	X	301	9/10	0.95	0.12	-	19,21,23,26	0
2	OZT	2	301	9/10	0.94	0.13	-	25,31,33,35	0
2	OZT	J	301	9/10	0.95	0.12	-	19,23,27,31	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	DMF	2	49	5/5	0.60	0.47	29.93	93,93,94,94	0
3	DMF	E	20	5/5	0.57	0.48	24.95	84,84,85,85	0
3	DMF	Z	18	5/5	0.68	0.45	24.43	97,98,98,99	0
3	DMF	P	14	5/5	0.60	0.53	21.89	90,91,92,92	0
3	DMF	G	24	5/5	0.70	0.44	20.29	80,80,81,82	0
3	DMF	T	29	5/5	0.89	0.30	18.46	63,63,63,63	0
3	DMF	V	27	5/5	0.92	0.33	16.16	77,77,78,79	0
3	DMF	Z	54	5/5	0.62	0.42	15.12	85,86,86,86	0
3	DMF	N	22	5/5	0.60	0.47	14.99	91,92,92,92	0
3	DMF	L	3	5/5	0.87	0.33	11.60	57,58,59,60	0
3	DMF	C	10	5/5	0.81	0.30	11.29	42,45,46,48	0
3	DMF	J	45	5/5	0.81	0.36	11.00	85,85,85,85	0
3	DMF	G	12	5/5	0.78	0.30	10.50	66,67,67,67	0
3	DMF	2	42	5/5	0.93	0.21	8.19	54,54,55,55	0
3	DMF	I	249	5/5	0.84	0.27	8.09	55,56,58,59	0
3	DMF	K	250	5/5	0.71	0.28	7.78	57,59,59,60	0
3	DMF	E	28	5/5	0.92	0.26	7.52	45,47,48,48	0
3	DMF	1	250	5/5	0.54	0.30	7.47	61,62,63,63	0
3	DMF	H	26	5/5	0.88	0.23	7.32	64,64,65,65	0
3	DMF	L	53	5/5	0.80	0.33	6.88	84,84,85,86	0
3	DMF	C	47	5/5	0.81	0.30	6.88	71,71,71,72	0
3	DMF	P	56	5/5	0.88	0.24	6.51	64,64,64,65	0
3	DMF	H	32	5/5	0.63	0.41	6.27	73,74,75,76	0
3	DMF	W	249	5/5	0.82	0.32	5.92	76,76,77,78	0
3	DMF	N	58	5/5	0.79	0.30	5.78	54,56,58,59	0
3	DMF	R	34	5/5	0.86	0.28	5.26	68,69,70,71	0
3	DMF	T	67	5/5	0.88	0.29	5.16	51,51,53,53	0
3	DMF	J	50	5/5	0.86	0.22	4.93	57,58,58,58	0
3	DMF	Z	30	5/5	0.92	0.20	4.55	56,56,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	DMF	G	60	5/5	0.89	0.27	4.49	50,52,52,52	0
3	DMF	M	249	5/5	0.86	0.26	4.45	54,54,55,56	0
3	DMF	E	66	5/5	0.74	0.30	4.32	65,65,66,67	0
3	DMF	G	1	5/5	0.94	0.21	4.25	42,44,45,46	0
3	DMF	B	250	5/5	0.82	0.28	4.06	77,78,78,79	0
3	DMF	K	251	5/5	0.88	0.27	3.99	60,62,62,62	0
3	DMF	J	4	5/5	0.85	0.26	3.77	60,61,61,62	0
3	DMF	O	249	5/5	0.92	0.23	3.09	46,47,48,50	0
3	DMF	X	61	5/5	0.89	0.22	3.08	55,56,58,60	0
3	DMF	M	250	5/5	0.89	0.18	2.63	39,40,41,41	0
3	DMF	U	249	5/5	0.94	0.20	2.59	51,51,52,52	0
3	DMF	S	249	5/5	0.90	0.23	2.58	79,80,81,81	0
3	DMF	X	16	5/5	0.91	0.20	2.56	46,46,47,48	0
3	DMF	L	36	5/5	0.94	0.21	2.47	57,57,58,58	0
3	DMF	N	15	5/5	0.95	0.17	2.44	44,46,47,47	0
3	DMF	G	64	5/5	0.81	0.27	2.43	56,57,58,58	0
3	DMF	D	249	5/5	0.93	0.20	2.39	53,53,53,54	0
3	DMF	R	59	5/5	0.89	0.24	2.28	58,59,60,60	0
3	DMF	2	52	5/5	0.86	0.26	2.17	75,75,76,76	0
3	DMF	C	55	5/5	0.86	0.24	2.12	74,74,74,74	0
3	DMF	P	51	5/5	0.79	0.32	2.11	76,76,76,76	0
3	DMF	P	65	5/5	0.88	0.22	1.96	50,51,52,52	0
3	DMF	1	249	5/5	0.89	0.20	1.95	49,51,51,52	0
3	DMF	H	62	5/5	0.90	0.22	1.72	42,43,45,47	0
3	DMF	A	249	5/5	0.89	0.19	1.70	60,61,62,62	0
3	DMF	K	249	5/5	0.93	0.19	1.66	51,53,54,55	0
3	DMF	B	249	5/5	0.94	0.20	1.57	47,47,48,48	0
3	DMF	F	249	5/5	0.90	0.20	1.54	70,71,71,71	0
3	DMF	I	250	5/5	0.93	0.17	0.98	61,61,61,61	0
3	DMF	H	33	5/5	0.93	0.18	0.72	39,40,41,41	0
3	DMF	2	63	5/5	0.94	0.17	0.53	43,45,45,46	0
3	DMF	Z	43	5/5	0.93	0.16	0.33	48,48,49,49	0
3	DMF	Q	249	5/5	0.91	0.16	0.27	49,49,50,50	0
3	DMF	Z	41	5/5	0.82	0.40	-	93,93,93,93	0
3	DMF	V	39	5/5	0.88	0.30	-	72,72,72,72	0
3	DMF	C	38	5/5	0.89	0.26	-	63,64,64,65	0
3	DMF	X	40	5/5	0.70	0.33	-	92,93,93,93	0
3	DMF	N	2	5/5	0.83	0.26	-	69,69,70,70	0

6.5 Other polymers [i](#)

There are no such residues in this entry.