Full wwPDB X-ray Structure Validation Report (i)

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 Full wwPDB X-ray Structure Validation 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

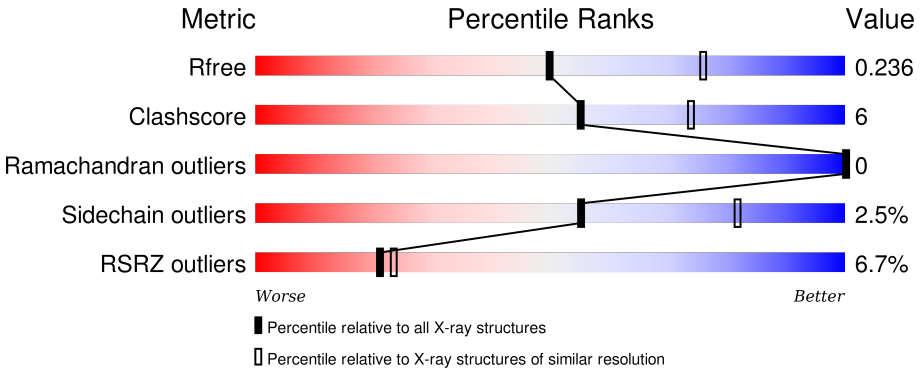
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.51 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	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 <=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	8% 77% 8% • 13%
1	A	248	10% 76% 10% • 13%
1	B	248	7% 78% 8% 14%
1	D	248	11% 75% 10% • 14%
1	F	248	6% 78% 8% 13%

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Mol	Chain	Length	Quality of chain
1	I	248	10% 75% 10% • 14%
1	K	248	16% 77% 9% • 13%
1	M	248	11% 74% 13% 13%
1	O	248	8% 76% 10% • 13%
1	Q	248	9% 72% 15% 13%
1	S	248	12% 75% 11% • 13%
1	U	248	8% 74% 11% • 14%
1	W	248	11% 76% 10% • 13%
1	Y	248	14% 74% 10% • 14%
2	2	240	3% 85% 5% 10%
2	C	240	2% 83% 6% 10%
2	E	240	82% 8% 10%
2	G	240	% 85% 5% 10%
2	H	240	% 82% 6% • 11%
2	J	240	3% 83% 8% 10%
2	L	240	2% 83% 7% 10%
2	N	240	% 81% 8% 11%
2	P	240	2% 84% 6% 10%
2	R	240	% 84% 8% • 7%
2	T	240	2% 83% 7% 10%
2	V	240	% 84% 9% 8%
2	X	240	2% 83% 7% 10%
2	Z	240	2% 83% 7% 10%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	DMF	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	C	N	O	S	0	0	0
			1593	998	274	317	4			
2	E	216	Total	C	N	O	S	0	0	0
			1601	1004	275	318	4			
2	G	216	Total	C	N	O	S	0	0	0
			1601	1004	275	318	4			
2	H	213	Total	C	N	O	S	0	0	0
			1583	992	272	315	4			
2	J	216	Total	C	N	O	S	0	0	0
			1601	1004	275	318	4			
2	L	216	Total	C	N	O	S	0	0	0
			1601	1004	275	318	4			
2	N	213	Total	C	N	O	S	0	0	0
			1580	989	272	315	4			
2	P	216	Total	C	N	O	S	0	0	0
			1601	1004	275	318	4			
2	R	223	Total	C	N	O	S	0	0	0
			1646	1031	282	329	4			
2	T	216	Total	C	N	O	S	0	0	0
			1601	1004	275	318	4			
2	V	222	Total	C	N	O	S	0	0	0
			1638	1025	281	328	4			
2	X	216	Total	C	N	O	S	0	0	0
			1601	1004	275	318	4			
2	Z	215	Total	C	N	O	S	0	0	0
			1593	998	274	317	4			
2	2	215	Total	C	N	O	S	0	0	0
			1593	998	274	317	4			

There are 98 discrepancies between the modelled and reference sequences:

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

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Chain	Residue	Modelled	Actual	Comment	Reference
E	539	HIS	-	EXPRESSION TAG	UNP O33245
E	540	HIS	-	EXPRESSION TAG	UNP O33245
G	301	OZT	-	INSERTION	UNP O33245
G	535	HIS	-	EXPRESSION TAG	UNP O33245
G	536	HIS	-	EXPRESSION TAG	UNP O33245
G	537	HIS	-	EXPRESSION TAG	UNP O33245
G	538	HIS	-	EXPRESSION TAG	UNP O33245
G	539	HIS	-	EXPRESSION TAG	UNP O33245
G	540	HIS	-	EXPRESSION TAG	UNP O33245
H	301	OZT	-	INSERTION	UNP O33245
H	535	HIS	-	EXPRESSION TAG	UNP O33245
H	536	HIS	-	EXPRESSION TAG	UNP O33245
H	537	HIS	-	EXPRESSION TAG	UNP O33245
H	538	HIS	-	EXPRESSION TAG	UNP O33245
H	539	HIS	-	EXPRESSION TAG	UNP O33245
H	540	HIS	-	EXPRESSION TAG	UNP O33245
J	301	OZT	-	INSERTION	UNP O33245
J	535	HIS	-	EXPRESSION TAG	UNP O33245
J	536	HIS	-	EXPRESSION TAG	UNP O33245
J	537	HIS	-	EXPRESSION TAG	UNP O33245
J	538	HIS	-	EXPRESSION TAG	UNP O33245
J	539	HIS	-	EXPRESSION TAG	UNP O33245
J	540	HIS	-	EXPRESSION TAG	UNP O33245
L	301	OZT	-	INSERTION	UNP O33245
L	535	HIS	-	EXPRESSION TAG	UNP O33245
L	536	HIS	-	EXPRESSION TAG	UNP O33245
L	537	HIS	-	EXPRESSION TAG	UNP O33245
L	538	HIS	-	EXPRESSION TAG	UNP O33245
L	539	HIS	-	EXPRESSION TAG	UNP O33245
L	540	HIS	-	EXPRESSION TAG	UNP O33245
N	301	OZT	-	INSERTION	UNP O33245
N	535	HIS	-	EXPRESSION TAG	UNP O33245
N	536	HIS	-	EXPRESSION TAG	UNP O33245
N	537	HIS	-	EXPRESSION TAG	UNP O33245
N	538	HIS	-	EXPRESSION TAG	UNP O33245
N	539	HIS	-	EXPRESSION TAG	UNP O33245
N	540	HIS	-	EXPRESSION TAG	UNP O33245
P	301	OZT	-	INSERTION	UNP O33245
P	535	HIS	-	EXPRESSION TAG	UNP O33245
P	536	HIS	-	EXPRESSION TAG	UNP O33245
P	537	HIS	-	EXPRESSION TAG	UNP O33245
P	538	HIS	-	EXPRESSION TAG	UNP O33245

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Chain	Residue	Modelled	Actual	Comment	Reference
P	539	HIS	-	EXPRESSION TAG	UNP O33245
P	540	HIS	-	EXPRESSION TAG	UNP O33245
R	301	OZT	-	INSERTION	UNP O33245
R	535	HIS	-	EXPRESSION TAG	UNP O33245
R	536	HIS	-	EXPRESSION TAG	UNP O33245
R	537	HIS	-	EXPRESSION TAG	UNP O33245
R	538	HIS	-	EXPRESSION TAG	UNP O33245
R	539	HIS	-	EXPRESSION TAG	UNP O33245
R	540	HIS	-	EXPRESSION TAG	UNP O33245
T	301	OZT	-	INSERTION	UNP O33245
T	535	HIS	-	EXPRESSION TAG	UNP O33245
T	536	HIS	-	EXPRESSION TAG	UNP O33245
T	537	HIS	-	EXPRESSION TAG	UNP O33245
T	538	HIS	-	EXPRESSION TAG	UNP O33245
T	539	HIS	-	EXPRESSION TAG	UNP O33245
T	540	HIS	-	EXPRESSION TAG	UNP O33245
V	301	OZT	-	INSERTION	UNP O33245
V	535	HIS	-	EXPRESSION TAG	UNP O33245
V	536	HIS	-	EXPRESSION TAG	UNP O33245
V	537	HIS	-	EXPRESSION TAG	UNP O33245
V	538	HIS	-	EXPRESSION TAG	UNP O33245
V	539	HIS	-	EXPRESSION TAG	UNP O33245
V	540	HIS	-	EXPRESSION TAG	UNP O33245
X	301	OZT	-	INSERTION	UNP O33245
X	535	HIS	-	EXPRESSION TAG	UNP O33245
X	536	HIS	-	EXPRESSION TAG	UNP O33245
X	537	HIS	-	EXPRESSION TAG	UNP O33245
X	538	HIS	-	EXPRESSION TAG	UNP O33245
X	539	HIS	-	EXPRESSION TAG	UNP O33245
X	540	HIS	-	EXPRESSION TAG	UNP O33245
Z	301	OZT	-	INSERTION	UNP O33245
Z	535	HIS	-	EXPRESSION TAG	UNP O33245
Z	536	HIS	-	EXPRESSION TAG	UNP O33245
Z	537	HIS	-	EXPRESSION TAG	UNP O33245
Z	538	HIS	-	EXPRESSION TAG	UNP O33245
Z	539	HIS	-	EXPRESSION TAG	UNP O33245
Z	540	HIS	-	EXPRESSION TAG	UNP O33245
2	301	OZT	-	INSERTION	UNP O33245
2	535	HIS	-	EXPRESSION TAG	UNP O33245
2	536	HIS	-	EXPRESSION TAG	UNP O33245
2	537	HIS	-	EXPRESSION TAG	UNP O33245
2	538	HIS	-	EXPRESSION TAG	UNP O33245

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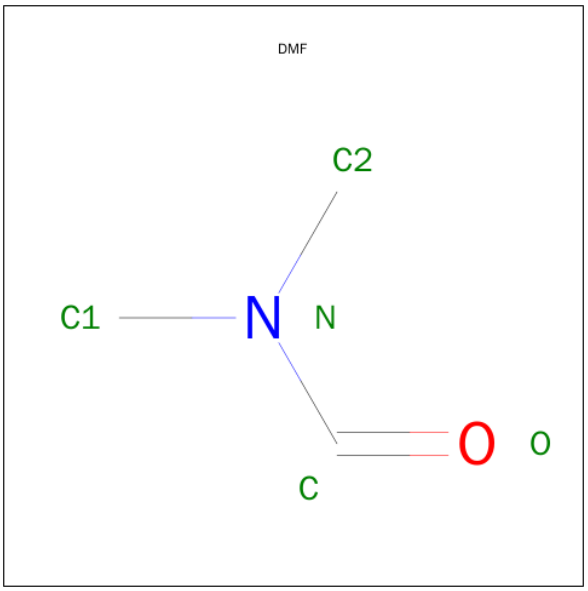
Chain	Residue	Modelled	Actual	Comment	Reference
2	539	HIS	-	EXPRESSION TAG	UNP O33245
2	540	HIS	-	EXPRESSION TAG	UNP O33245

- Molecule 3 is DIMETHYLFORMAMIDE (three-letter code: DMF) (formula: C_3H_7NO).



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

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

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

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	W	1	Total	C	N	O	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	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 O 89 89	0	0
4	F	40	Total O 40 40	0	0
4	G	72	Total O 72 72	0	0
4	H	91	Total O 91 91	0	0
4	I	38	Total O 38 38	0	0
4	J	90	Total O 90 90	0	0
4	K	39	Total O 39 39	0	0
4	L	90	Total O 90 90	0	0
4	M	42	Total O 42 42	0	0
4	N	86	Total O 86 86	0	0
4	O	40	Total O 40 40	0	0
4	P	82	Total O 82 82	0	0
4	Q	34	Total O 34 34	0	0
4	R	97	Total O 97 97	0	0
4	S	34	Total O 34 34	0	0
4	T	78	Total O 78 78	0	0
4	U	38	Total O 38 38	0	0
4	V	104	Total O 104 104	0	0
4	W	27	Total O 27 27	0	0
4	X	84	Total O 84 84	0	0
4	Y	24	Total O 24 24	0	0

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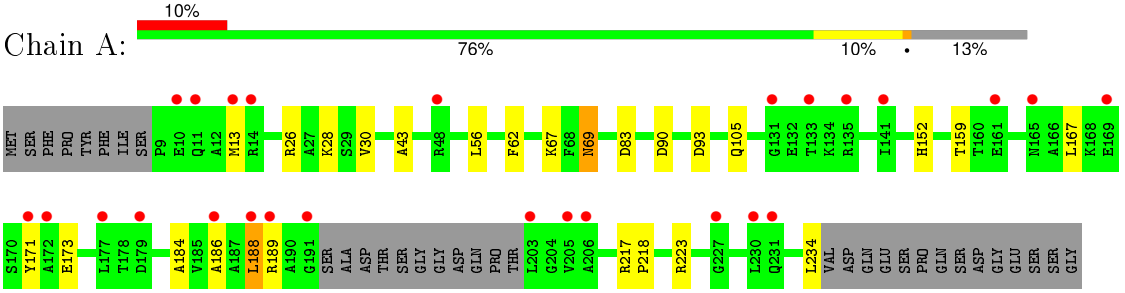
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	Z	85	Total O 85 85	0	0
4	1	34	Total O 34 34	0	0
4	2	93	Total O 93 93	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA 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.

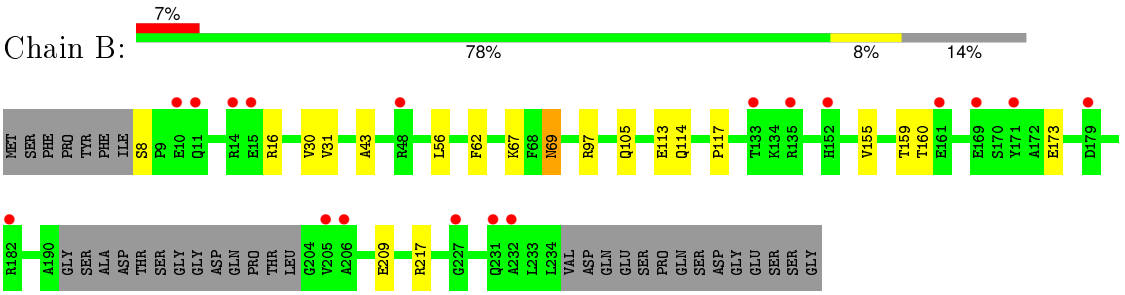
- Molecule 1: Proteasome (Alpha subunit) PrcA

Chain A:



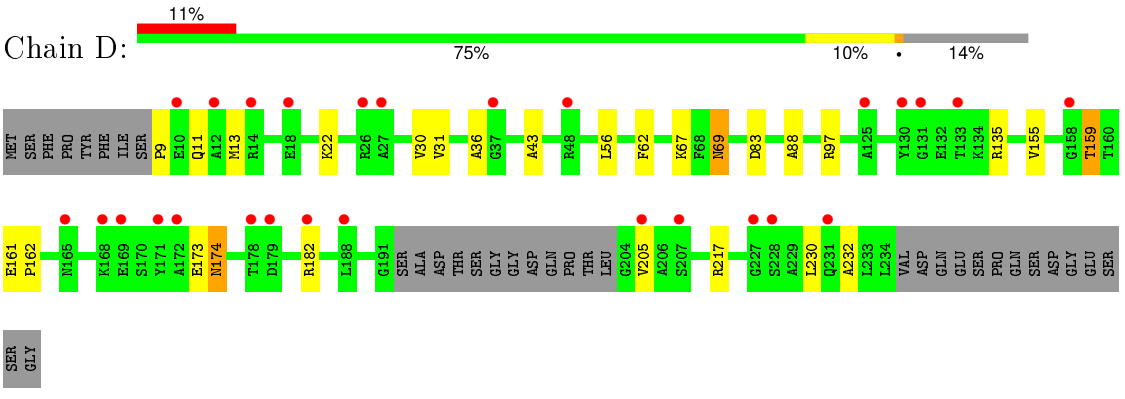
- Molecule 1: Proteasome (Alpha subunit) PrcA

Chain B:



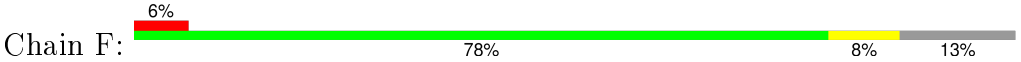
- Molecule 1: Proteasome (Alpha subunit) PrcA

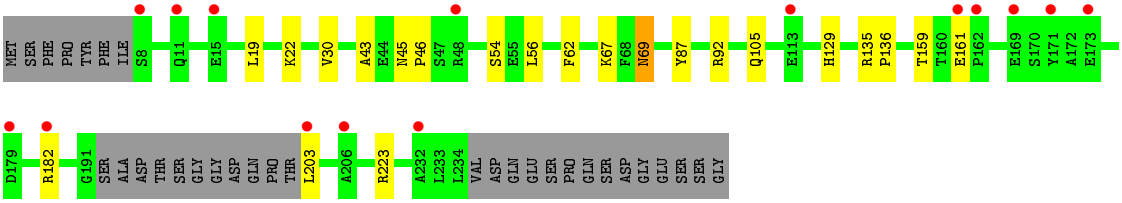
Chain D:



- Molecule 1: Proteasome (Alpha subunit) PrcA

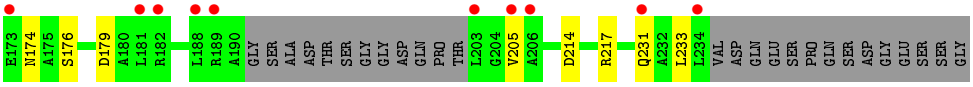
Chain F:





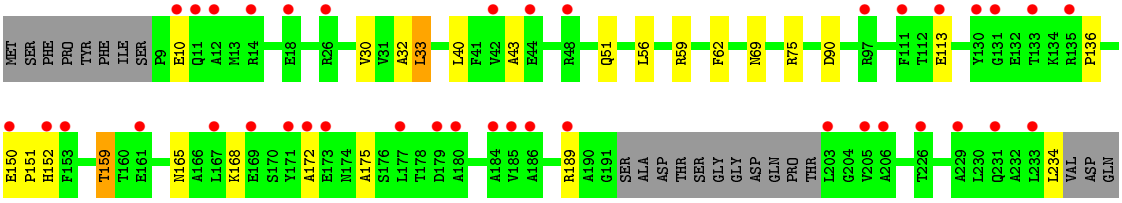
• Molecule 1: Proteasome (Alpha subunit) PrcA

Chain I:



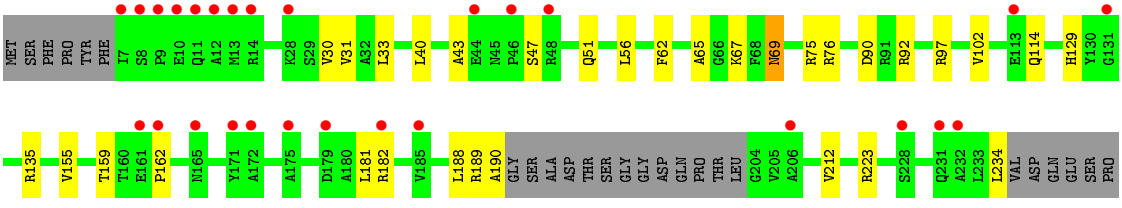
• Molecule 1: Proteasome (Alpha subunit) PrcA

Chain K:



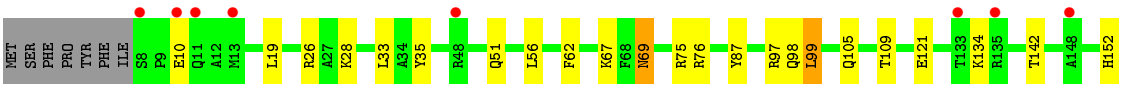
• Molecule 1: Proteasome (Alpha subunit) PrcA

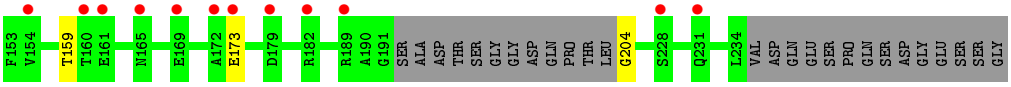
Chain M:



• Molecule 1: Proteasome (Alpha subunit) PrcA

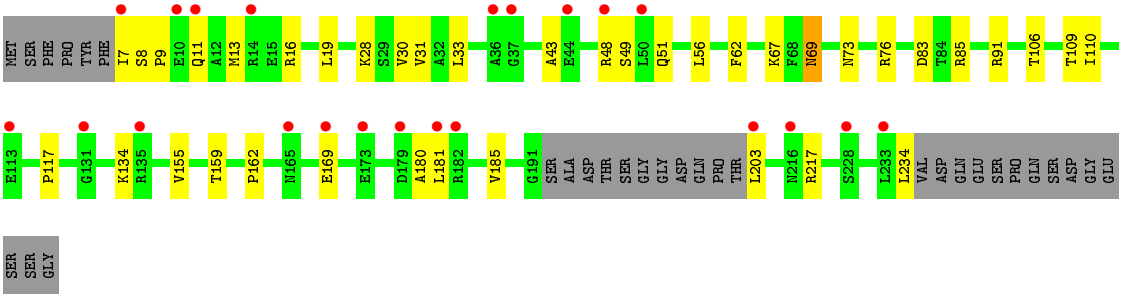
Chain O:





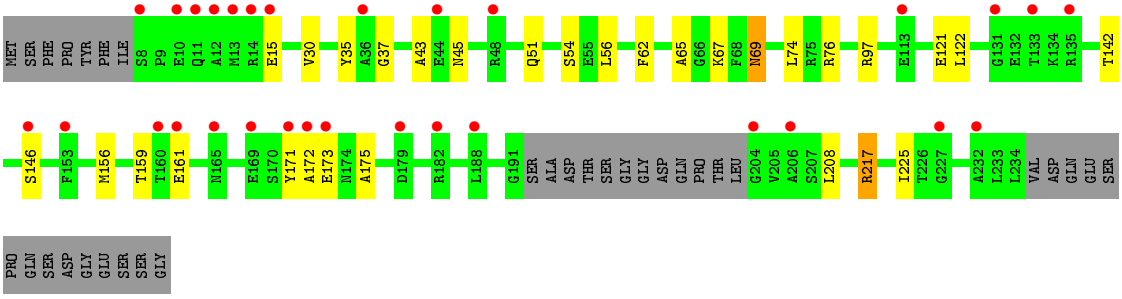
• Molecule 1: Proteasome (Alpha subunit) PrcA

Chain Q:



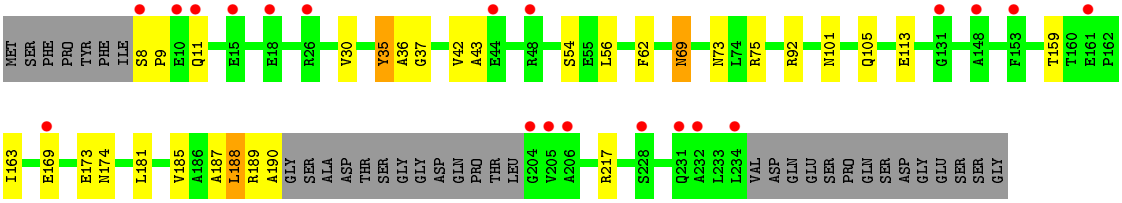
• Molecule 1: Proteasome (Alpha subunit) PrcA

Chain S:



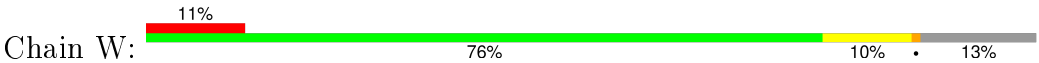
• Molecule 1: Proteasome (Alpha subunit) PrcA

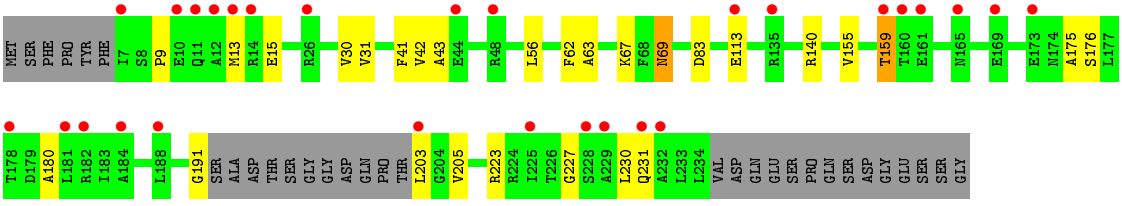
Chain U:



• Molecule 1: Proteasome (Alpha subunit) PrcA

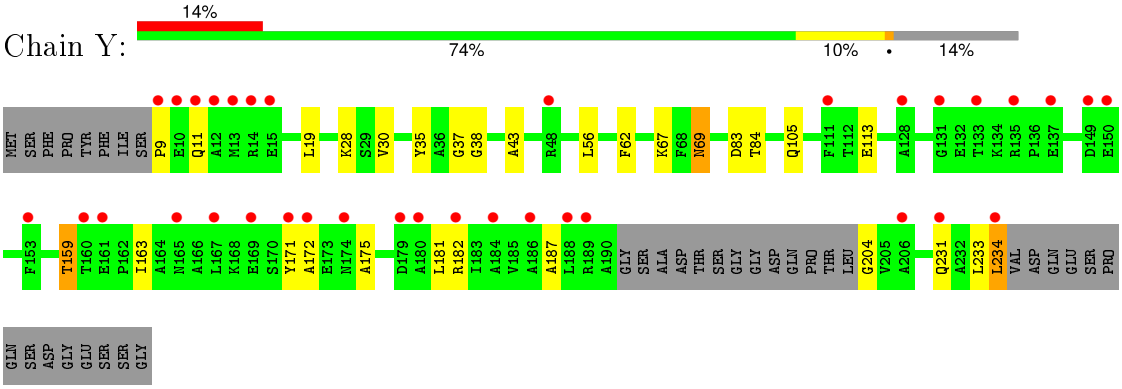
Chain W:





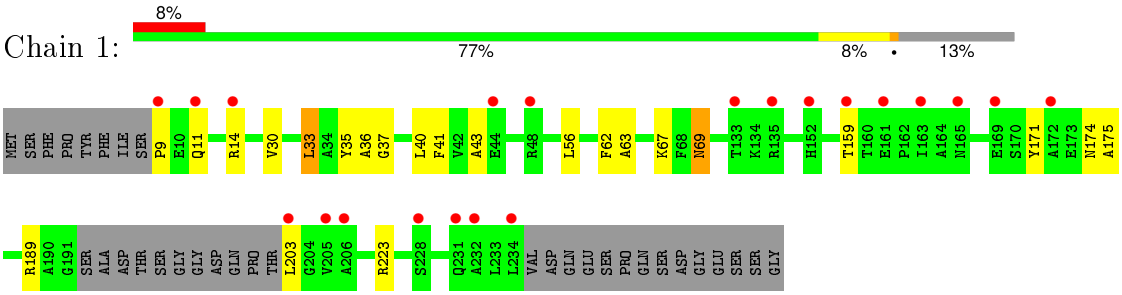
• Molecule 1: Proteasome (Alpha subunit) PrcA

Chain Y:



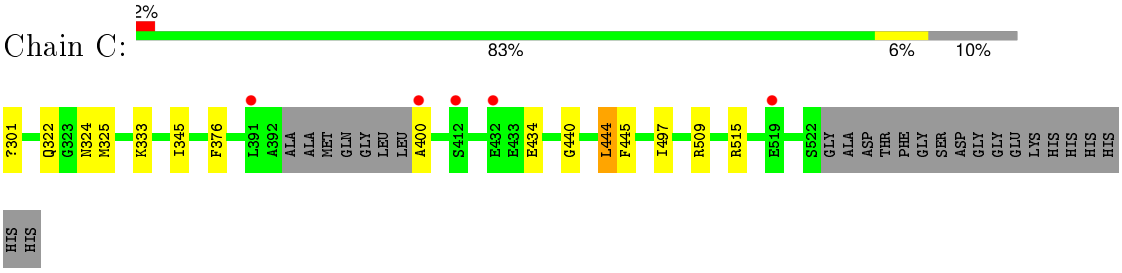
• Molecule 1: Proteasome (Alpha subunit) PrcA

Chain 1:



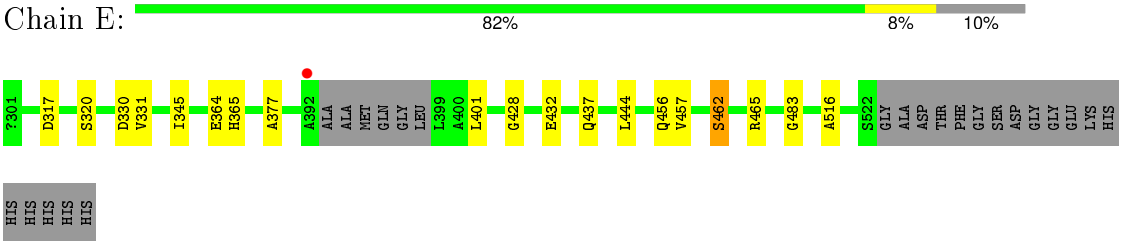
• Molecule 2: Proteasome (Beta subunit) PrcB

Chain C:



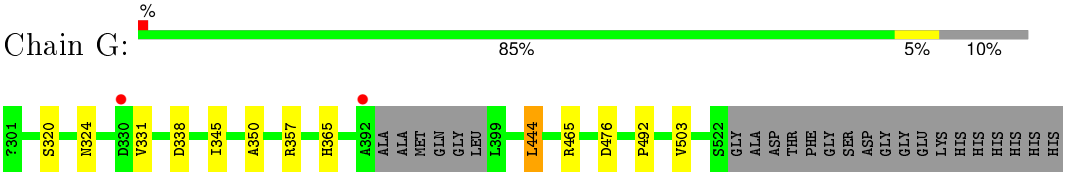
• Molecule 2: Proteasome (Beta subunit) PrcB

Chain E:



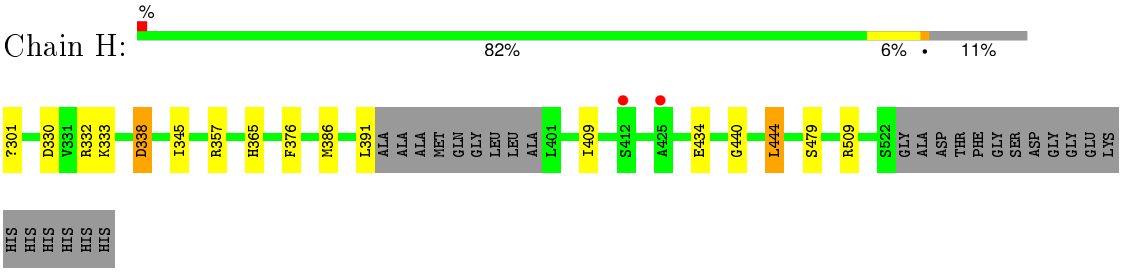
• Molecule 2: Proteasome (Beta subunit) PrcB

Chain G:



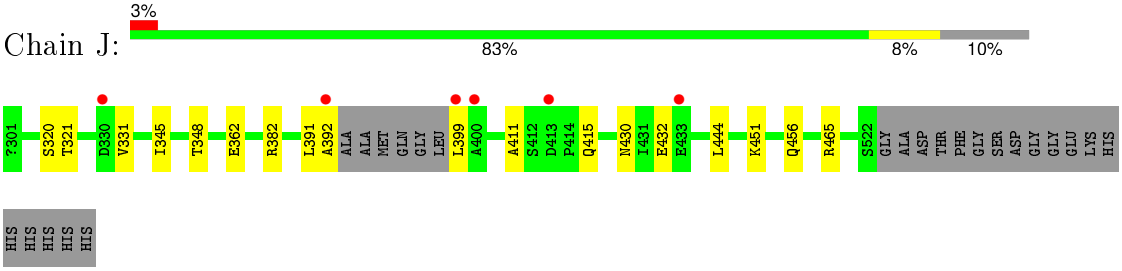
• Molecule 2: Proteasome (Beta subunit) PrcB

Chain H:



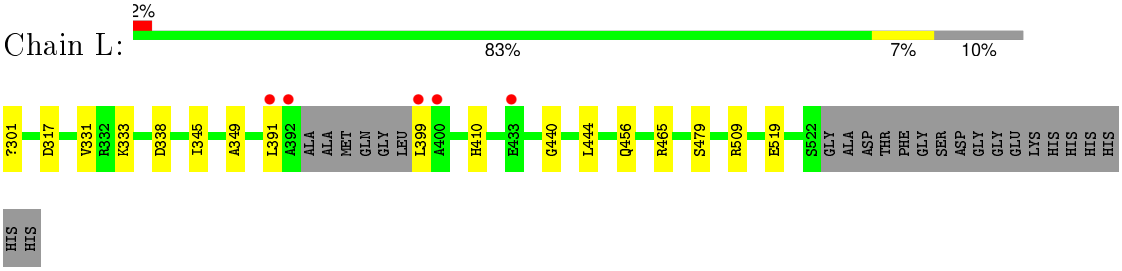
• Molecule 2: Proteasome (Beta subunit) PrcB

Chain J:



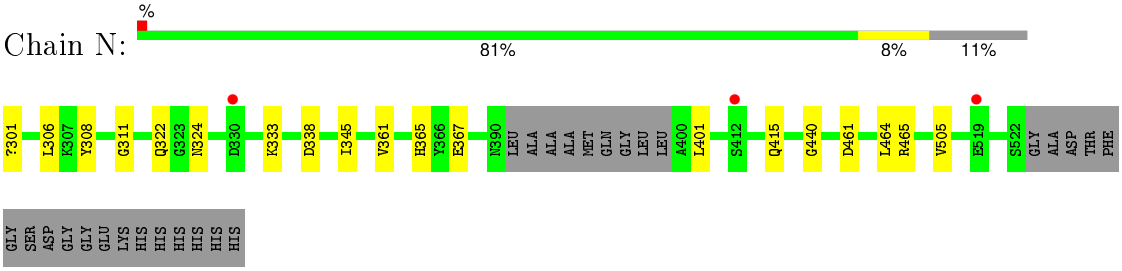
• Molecule 2: Proteasome (Beta subunit) PrcB

Chain L:



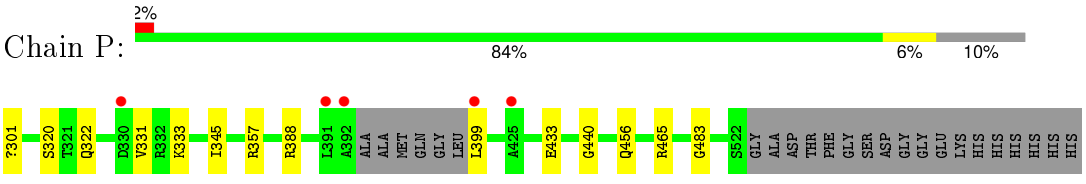
• Molecule 2: Proteasome (Beta subunit) PrcB

Chain N:



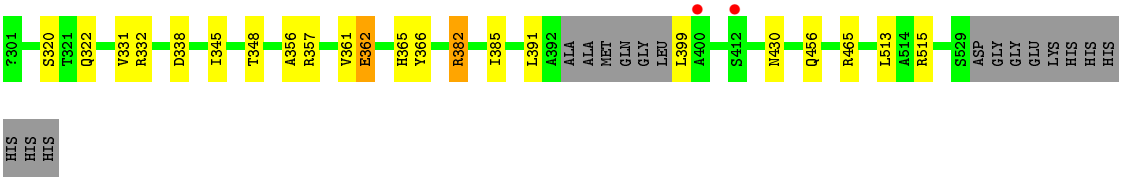
• Molecule 2: Proteasome (Beta subunit) PrcB

Chain P:



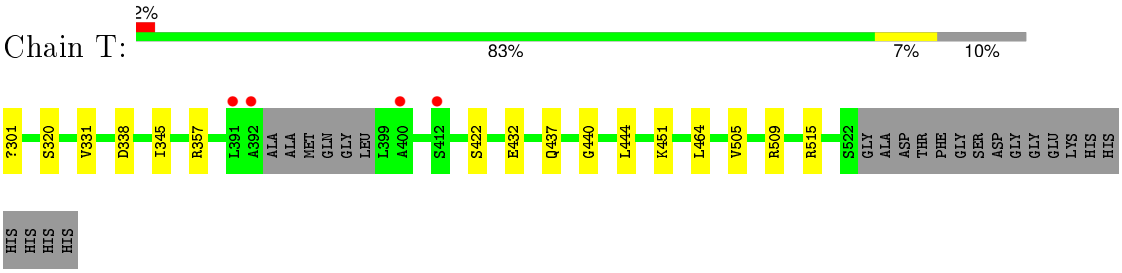
• Molecule 2: Proteasome (Beta subunit) PrcB

Chain R:



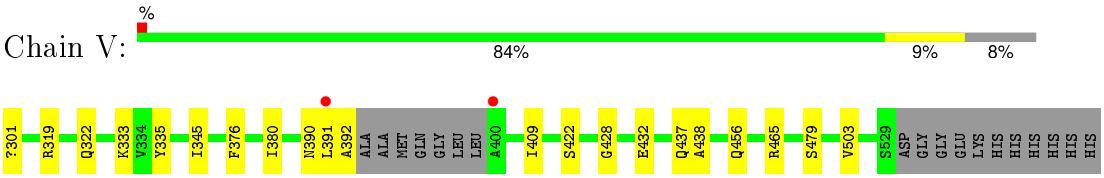
- Molecule 2: Proteasome (Beta subunit) PrcB

Chain T:



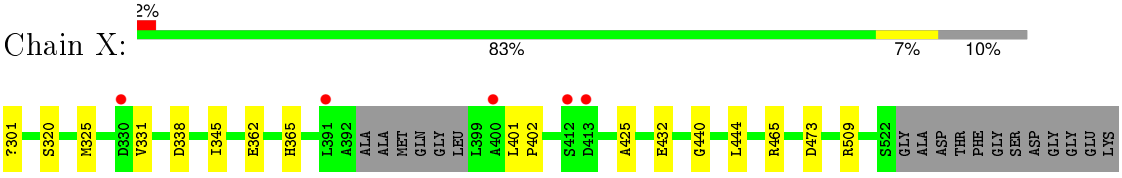
- Molecule 2: Proteasome (Beta subunit) PrcB

Chain V:



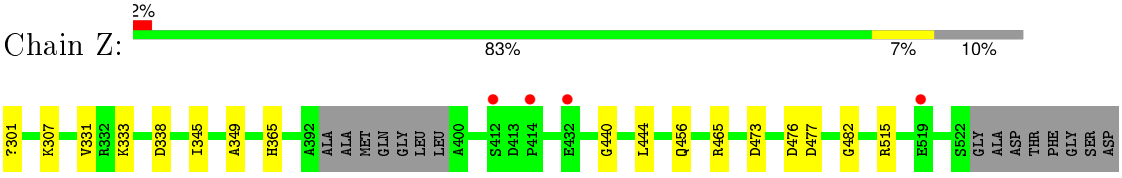
- Molecule 2: Proteasome (Beta subunit) PrcB

Chain X:



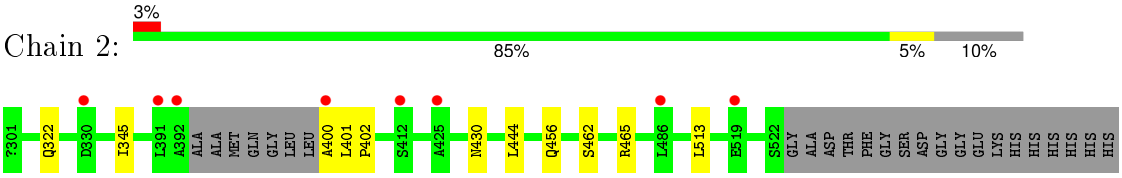
- Molecule 2: Proteasome (Beta subunit) PrcB

Chain Z:



- Molecule 2: Proteasome (Beta subunit) PrcB

Chain 2:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	171.98Å 118.04Å 197.06Å 90.00° 113.62° 90.00°	Depositor
Resolution (Å)	29.83 – 2.51 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
$< I/\sigma(I) >$ [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]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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(^{o})	Ideal(^{o})
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.

All (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
1:I:135:ARG:HG2	4:I:1769:HOH:O	1.39	1.17
4:A:1674:HOH:O	1:B:8:SER:HB2	1.45	1.16
1:Y:182:ARG:HD3	4:Y:1675:HOH:O	1.42	1.15
1:O:121:GLU:HG3	4:O:1391:HOH:O	1.41	1.15
2:X:401:LEU:HB2	4:X:1614:HOH:O	1.42	1.14

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:515:ARG:HD3	4:T:1499:HOH:O	1.44	1.14
1:Y:233:LEU:O	1:Y:234:LEU:O	1.69	1.11
1:K:168:LYS:HD2	4:K:1705:HOH:O	1.53	1.08
1:K:189:ARG:HD2	4:K:1741:HOH:O	1.51	1.08
1:W:159:THR:HB	4:W:1559:HOH:O	1.53	1.08
2:H:332:ARG:HB2	4:H:1570:HOH:O	1.53	1.07
1:U:9:PRO:HD3	4:U:1536:HOH:O	1.56	1.06
1:B:173:GLU:HG3	4:B:1646:HOH:O	1.52	1.05
2:J:399:LEU:HG	4:J:1403:HOH:O	1.54	1.04
1:Q:134:LYS:HE3	4:Q:1565:HOH:O	1.53	1.03
1:M:223:ARG:HD3	4:M:1627:HOH:O	1.60	1.01
4:F:1688:HOH:O	1:W:9:PRO:HG3	1.58	1.00
1:M:223:ARG:HG2	4:M:1631:HOH:O	1.61	1.00
2:C:400:ALA:HB2	4:C:1575:HOH:O	1.62	1.00
1:A:186:ALA:O	1:A:189:ARG:HG2	1.60	0.99
2:H:332:ARG:HD2	4:H:1570:HOH:O	1.61	0.99
1:Y:28:LYS:HE3	4:Y:1700:HOH:O	1.61	0.99
1:U:92:ARG:HB2	4:U:1709:HOH:O	1.63	0.99
3:X:40:DMF:H22	4:X:1639:HOH:O	1.62	0.98
1:A:152:HIS:HB3	1:A:171:TYR:CE2	2.00	0.97
1:D:173:GLU:C	1:D:174:ASN:ND2	2.19	0.95
1:O:26:ARG:HG3	4:O:1474:HOH:O	1.67	0.95
2:V:456:GLN:HE21	2:V:465:ARG:HH22	1.13	0.94
1:A:26:ARG:HD3	4:A:1777:HOH:O	1.69	0.91
1:M:182:ARG:HD3	4:M:1510:HOH:O	1.68	0.91
2:J:456:GLN:HE21	2:J:465:ARG:HH22	1.18	0.89
4:M:1478:HOH:O	2:N:361:VAL:HG23	1.74	0.88
1:U:217:ARG:HD3	4:U:1532:HOH:O	1.74	0.87
4:K:1467:HOH:O	1:M:97:ARG:HD2	1.74	0.87
2:T:357:ARG:HD2	4:T:1567:HOH:O	1.72	0.87
1:O:76:ARG:HD3	4:O:1375:HOH:O	1.74	0.86
2:C:324:ASN:HB2	4:C:1648:HOH:O	1.72	0.86
2:X:465:ARG:HD2	4:X:1379:HOH:O	1.75	0.86
1:D:173:GLU:HG2	1:D:174:ASN:ND2	1.91	0.85
2:J:399:LEU:HD12	4:J:1413:HOH:O	1.75	0.85
2:2:430:ASN:HB2	4:2:1473:HOH:O	1.76	0.85
1:Y:35:TYR:CD2	1:Y:38:GLY:O	2.29	0.85
1:Y:181:LEU:HD12	1:Y:233:LEU:HD22	1.56	0.85
1:S:225:ILE:HA	4:S:1371:HOH:O	1.75	0.84
1:1:14:ARG:HA	4:1:1788:HOH:O	1.77	0.84
1:S:217:ARG:HD2	4:S:1458:HOH:O	1.76	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:182:ARG:HB2	4:M:1510:HOH:O	1.77	0.84
1:B:105:GLN:HG3	4:B:1554:HOH:O	1.78	0.84
1:D:173:GLU:CG	1:D:174:ASN:HD21	1.90	0.84
1:O:26:ARG:CD	4:O:1474:HOH:O	2.25	0.83
2:L:410:HIS:CE1	4:L:1630:HOH:O	2.31	0.83
1:1:14:ARG:HG2	4:1:1448:HOH:O	1.76	0.83
1:I:9:PRO:HD3	4:I:1373:HOH:O	1.79	0.83
1:Q:7:ILE:HG23	1:Q:11:GLN:HB3	1.59	0.83
2:X:432:GLU:HG2	4:X:1310:HOH:O	1.80	0.82
1:I:92:ARG:HD2	4:I:1723:HOH:O	1.77	0.82
1:U:181:LEU:O	1:U:185:VAL:HG23	1.79	0.82
1:U:69:ASN:H	1:U:69:ASN:HD22	1.26	0.81
3:J:4:DMF:C2	4:J:1466:HOH:O	2.28	0.81
1:1:14:ARG:CG	4:1:1788:HOH:O	2.28	0.81
4:M:1478:HOH:O	2:N:361:VAL:CG2	2.28	0.80
1:B:97:ARG:HD2	4:B:1748:HOH:O	1.82	0.80
1:K:33:LEU:CD1	1:K:33:LEU:O	2.30	0.80
2:T:509:ARG:HD2	4:T:1578:HOH:O	1.81	0.80
2:V:456:GLN:NE2	2:V:465:ARG:HH22	1.78	0.80
1:D:174:ASN:N	1:D:174:ASN:ND2	2.30	0.79
1:B:97:ARG:CD	4:B:1748:HOH:O	2.29	0.79
1:D:232:ALA:HB2	4:D:1728:HOH:O	1.81	0.79
1:B:217:ARG:CD	4:B:1475:HOH:O	2.31	0.79
2:P:456:GLN:HE21	2:P:465:ARG:HH12	1.27	0.79
1:W:231:GLN:HA	4:W:1447:HOH:O	1.82	0.79
1:D:36:ALA:HB3	4:D:1680:HOH:O	1.81	0.79
1:1:171:TYR:CE1	4:1:1654:HOH:O	2.36	0.79
2:2:444:LEU:CD1	4:2:1592:HOH:O	2.30	0.79
1:K:136:PRO:HD3	4:K:1568:HOH:O	1.82	0.78
1:Y:231:GLN:HA	4:Y:1576:HOH:O	1.83	0.78
2:J:321:THR:H	3:J:4:DMF:HC	1.48	0.78
2:G:444:LEU:HB3	4:G:1370:HOH:O	1.83	0.78
2:2:456:GLN:HE22	2:2:465:ARG:HH22	1.31	0.78
1:A:26:ARG:CD	4:A:1777:HOH:O	2.28	0.77
2:V:456:GLN:HE22	2:V:465:ARG:HH12	1.32	0.77
1:1:223:ARG:CD	4:1:1596:HOH:O	2.32	0.77
1:B:217:ARG:HD3	4:B:1475:HOH:O	1.85	0.77
1:B:160:THR:HG22	4:B:1526:HOH:O	1.84	0.77
1:1:33:LEU:HD12	1:1:40:LEU:HB3	1.67	0.76
1:D:173:GLU:CG	1:D:174:ASN:ND2	2.48	0.76
2:J:444:LEU:HB3	4:J:1376:HOH:O	1.84	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:14:ARG:HG3	4:1:1788:HOH:O	1.86	0.75
1:1:223:ARG:HD3	4:1:1596:HOH:O	1.86	0.75
1:O:26:ARG:CG	4:O:1474:HOH:O	2.28	0.75
1:D:173:GLU:CB	1:D:174:ASN:ND2	2.49	0.75
3:T:29:DMF:H22	4:T:1567:HOH:O	1.86	0.75
1:I:92:ARG:CD	4:I:1723:HOH:O	2.34	0.74
1:Y:181:LEU:CD1	1:Y:233:LEU:HD22	2.16	0.74
1:F:54:SER:HA	4:F:1410:HOH:O	1.87	0.74
1:Q:91:ARG:HD2	4:Q:1398:HOH:O	1.88	0.74
1:O:56:LEU:HD13	1:O:99:LEU:HD22	1.70	0.73
2:C:445:PHE:CE2	3:C:55:DMF:H12	2.23	0.73
1:S:121:GLU:HG3	4:S:1386:HOH:O	1.88	0.73
1:Y:234:LEU:HD23	1:Y:234:LEU:C	2.08	0.73
1:K:33:LEU:HD12	1:K:33:LEU:O	1.88	0.73
1:O:134:LYS:HB2	4:O:1785:HOH:O	1.87	0.73
1:D:173:GLU:HG2	1:D:174:ASN:HD21	1.49	0.73
1:F:182:ARG:HB2	4:F:1672:HOH:O	1.88	0.73
1:K:136:PRO:HG3	4:K:1568:HOH:O	1.89	0.72
1:A:152:HIS:HB3	1:A:171:TYR:HE2	1.49	0.72
1:U:35:TYR:CE1	1:U:37:GLY:N	2.56	0.72
2:R:456:GLN:HE21	2:R:465:ARG:HH12	1.35	0.72
1:U:11:GLN:HG2	4:U:1729:HOH:O	1.89	0.72
2:H:376:PHE:HD1	4:H:1358:HOH:O	1.72	0.72
1:K:136:PRO:CD	4:K:1568:HOH:O	2.36	0.72
3:J:4:DMF:H21	4:J:1466:HOH:O	1.87	0.72
1:Y:181:LEU:HD12	1:Y:233:LEU:CD2	2.19	0.72
1:S:142:THR:HA	4:S:1386:HOH:O	1.90	0.71
4:D:1754:HOH:O	1:K:10:GLU:HG3	1.91	0.71
1:I:33:LEU:HD11	1:I:40:LEU:HD23	1.73	0.71
2:V:432:GLU:CD	2:V:437:GLN:HE21	1.95	0.71
1:Q:7:ILE:HG22	1:Q:8:SER:N	2.06	0.70
2:C:434:GLU:HG3	4:J:1791:HOH:O	1.89	0.70
1:O:105:GLN:OE1	1:U:73:ASN:HB2	1.91	0.70
1:F:92:ARG:CD	4:F:1747:HOH:O	2.39	0.70
1:S:97:ARG:CB	4:S:1727:HOH:O	2.38	0.70
1:O:134:LYS:HD2	4:O:1785:HOH:O	1.92	0.69
2:N:324:ASN:HB2	4:N:1388:HOH:O	1.92	0.69
1:Y:159:THR:HG23	4:Y:1427:HOH:O	1.92	0.69
1:Q:106:THR:O	1:Q:110:ILE:HG13	1.92	0.69
2:2:444:LEU:HD12	4:2:1592:HOH:O	1.92	0.68
1:W:227:GLY:HA3	4:W:1758:HOH:O	1.91	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:233:LEU:O	1:Y:234:LEU:C	2.30	0.68
2:V:456:GLN:HE21	2:V:465:ARG:NH2	1.89	0.68
2:X:425:ALA:HB2	4:X:1655:HOH:O	1.93	0.68
1:K:172:ALA:HB3	1:K:175:ALA:HB2	1.76	0.68
1:M:223:ARG:CD	4:M:1627:HOH:O	2.28	0.68
2:2:456:GLN:NE2	2:2:465:ARG:HH22	1.91	0.68
1:D:159:THR:HG22	4:D:1455:HOH:O	1.92	0.68
1:Y:84:THR:HB	4:Y:1479:HOH:O	1.94	0.68
1:1:33:LEU:CD1	1:1:40:LEU:HB3	2.24	0.68
1:M:162:PRO:HB2	1:M:190:ALA:O	1.94	0.67
1:S:35:TYR:CE1	1:S:37:GLY:HA3	2.29	0.67
1:S:15:GLU:OE2	1:1:9:PRO:HB3	1.95	0.67
2:L:410:HIS:ND1	4:L:1630:HOH:O	2.27	0.67
1:Q:73:ASN:ND2	4:Q:1696:HOH:O	2.27	0.67
1:I:176:SER:OG	1:I:179:ASP:HB2	1.95	0.67
2:J:456:GLN:NE2	2:J:465:ARG:HH22	1.90	0.67
1:O:10:GLU:HG3	4:O:1774:HOH:O	1.93	0.67
4:F:1702:HOH:O	2:G:365:HIS:HE1	1.77	0.66
2:R:456:GLN:NE2	2:R:465:ARG:HH22	1.94	0.66
2:C:325:MET:HE3	4:C:1776:HOH:O	1.95	0.66
1:Q:33:LEU:HD11	1:Q:180:ALA:HB1	1.78	0.66
1:M:33:LEU:HD12	1:M:33:LEU:O	1.96	0.66
1:Y:233:LEU:C	1:Y:234:LEU:O	2.35	0.66
1:D:11:GLN:HG2	4:D:1284:HOH:O	1.96	0.65
1:B:97:ARG:NE	4:B:1748:HOH:O	2.29	0.65
2:H:357:ARG:HD2	4:H:1224:HOH:O	1.96	0.65
1:I:217:ARG:NH1	4:I:1658:HOH:O	2.30	0.65
1:A:217:ARG:NH1	4:A:1792:HOH:O	2.30	0.65
2:Z:482:GLY:HA3	4:Z:1417:HOH:O	1.95	0.65
1:K:33:LEU:HD13	1:K:33:LEU:O	1.96	0.65
2:J:399:LEU:CD1	4:J:1413:HOH:O	2.40	0.65
1:Q:7:ILE:HG23	1:Q:11:GLN:CB	2.27	0.65
1:S:156:MET:HA	4:S:1513:HOH:O	1.94	0.65
1:K:33:LEU:CD1	1:K:40:LEU:HB3	2.26	0.65
1:M:223:ARG:CG	4:M:1631:HOH:O	2.32	0.65
1:Y:105:GLN:NE2	4:Y:1749:HOH:O	2.30	0.65
1:O:33:LEU:O	1:O:33:LEU:HD12	1.96	0.65
1:W:191:GLY:HA3	4:W:1559:HOH:O	1.97	0.64
1:D:9:PRO:HD3	1:Q:7:ILE:CD1	2.27	0.64
1:K:152:HIS:CG	4:K:1560:HOH:O	2.50	0.64
2:C:445:PHE:CD2	3:C:55:DMF:H12	2.33	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:456:GLN:HE22	2:R:465:ARG:HH22	1.45	0.64
1:F:92:ARG:HD2	4:F:1747:HOH:O	1.97	0.64
2:R:430:ASN:HB2	4:R:1290:HOH:O	1.98	0.64
2:Z:515:ARG:NE	4:Z:1691:HOH:O	2.30	0.64
4:F:1688:HOH:O	1:W:9:PRO:CG	2.30	0.64
2:J:451:LYS:NZ	2:Z:473:ASP:OD1	2.30	0.64
1:K:136:PRO:CG	4:K:1568:HOH:O	2.46	0.64
3:Z:18:DMF:C	4:Z:1771:HOH:O	2.46	0.64
1:F:161:GLU:N	1:F:161:GLU:OE1	2.30	0.64
1:F:19:LEU:HD11	1:W:13:MET:HG3	1.79	0.63
2:C:325:MET:CE	4:C:1776:HOH:O	2.45	0.63
1:U:69:ASN:H	1:U:69:ASN:ND2	1.91	0.63
2:H:444:LEU:HB3	4:H:1361:HOH:O	1.98	0.63
1:B:114:GLN:NE2	4:B:1389:HOH:O	2.29	0.63
1:S:172:ALA:HB3	1:S:175:ALA:HB2	1.80	0.62
2:H:409:ILE:CD1	4:H:1704:HOH:O	2.46	0.62
1:U:35:TYR:CE1	1:U:37:GLY:CA	2.83	0.62
1:Q:83:ASP:OD2	2:R:365:HIS:HD2	1.83	0.62
1:I:11:GLN:HB3	4:I:1368:HOH:O	2.00	0.62
2:H:434:GLU:HG3	4:H:1573:HOH:O	1.99	0.61
1:D:173:GLU:HB3	1:D:174:ASN:ND2	2.14	0.61
1:S:97:ARG:HB3	4:S:1727:HOH:O	1.99	0.61
1:O:152:HIS:CD2	1:O:173:GLU:OE2	2.52	0.61
1:Y:172:ALA:HB3	1:Y:175:ALA:HB2	1.82	0.61
1:O:28:LYS:HE3	4:O:1486:HOH:O	2.01	0.61
3:T:29:DMF:H21	4:T:1461:HOH:O	2.00	0.61
1:M:182:ARG:CG	4:M:1510:HOH:O	2.48	0.61
1:Q:28:LYS:HE3	4:Q:1387:HOH:O	1.99	0.61
1:O:33:LEU:HD12	1:O:33:LEU:C	2.22	0.60
1:A:184:ALA:O	1:A:188:LEU:HB2	2.01	0.60
2:2:400:ALA:HA	4:2:1459:HOH:O	2.01	0.60
4:M:1390:HOH:O	2:N:365:HIS:HE1	1.82	0.60
1:Q:7:ILE:CG2	1:Q:11:GLN:HB3	2.31	0.60
2:P:456:GLN:HE21	2:P:465:ARG:NH1	1.98	0.60
1:S:97:ARG:HD3	4:S:1727:HOH:O	2.02	0.60
1:Y:35:TYR:CE1	1:Y:37:GLY:HA3	2.36	0.60
2:N:401:LEU:HB2	4:N:1641:HOH:O	2.01	0.60
1:U:217:ARG:CD	4:U:1532:HOH:O	2.39	0.60
2:R:456:GLN:NE2	2:R:465:ARG:HH12	2.00	0.60
1:M:31:VAL:HG12	1:M:155:VAL:HG22	1.83	0.60
1:S:76:ARG:HD3	4:S:1020:HOH:O	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:7:ILE:CG2	1:Q:8:SER:N	2.64	0.60
2:X:425:ALA:CB	4:X:1655:HOH:O	2.47	0.60
2:X:509:ARG:NH1	4:X:1515:HOH:O	2.35	0.59
1:O:26:ARG:HD3	4:O:1474:HOH:O	1.98	0.59
1:D:36:ALA:CB	4:D:1680:HOH:O	2.44	0.59
1:F:56:LEU:HG	1:F:62:PHE:HB2	1.84	0.59
1:U:35:TYR:CD1	1:U:37:GLY:N	2.60	0.59
1:I:33:LEU:O	1:I:33:LEU:HD12	2.02	0.59
2:N:367:GLU:HG2	4:N:1520:HOH:O	2.01	0.59
1:Y:35:TYR:CZ	1:Y:37:GLY:HA3	2.38	0.59
1:1:223:ARG:HD2	4:1:1596:HOH:O	1.99	0.59
1:O:10:GLU:CG	4:O:1774:HOH:O	2.48	0.58
1:Q:48:ARG:CB	4:Q:1636:HOH:O	2.50	0.58
1:1:35:TYR:CE1	1:1:37:GLY:HA3	2.38	0.58
2:2:456:GLN:HE21	2:2:465:ARG:HH12	1.51	0.58
2:R:356:ALA:HB3	3:R:34:DMF:H22	1.86	0.58
1:Q:109:THR:HB	4:Q:1637:HOH:O	2.03	0.58
1:U:101:ASN:O	1:U:105:GLN:HG2	2.03	0.58
1:Q:7:ILE:N	4:Q:1206:HOH:O	2.36	0.57
2:V:409:ILE:HG22	4:V:1453:HOH:O	2.03	0.57
2:E:456:GLN:HE21	2:E:465:ARG:NH1	2.02	0.57
1:U:35:TYR:CE1	1:U:37:GLY:HA3	2.39	0.57
2:V:456:GLN:NE2	2:V:465:ARG:HH12	2.00	0.57
1:I:161:GLU:N	1:I:161:GLU:OE1	2.30	0.57
3:T:29:DMF:HC	4:T:1461:HOH:O	2.04	0.57
1:K:33:LEU:HD11	1:K:40:LEU:HB3	1.86	0.57
1:K:159:THR:HA	4:K:1652:HOH:O	2.05	0.57
1:Q:7:ILE:HG23	1:Q:11:GLN:CG	2.35	0.56
1:M:162:PRO:CB	1:M:190:ALA:O	2.53	0.56
1:A:28:LYS:HE3	4:A:1366:HOH:O	2.04	0.56
1:M:182:ARG:CD	4:M:1510:HOH:O	2.35	0.56
2:P:456:GLN:NE2	2:P:465:ARG:HH12	2.01	0.56
2:V:301:OZT:H27	2:V:333:LYS:HE2	1.86	0.56
1:B:217:ARG:HD2	4:B:1475:HOH:O	1.98	0.56
2:V:319:ARG:NH1	2:V:479:SER:O	2.38	0.56
2:J:415:GLN:HB3	4:J:1632:HOH:O	2.04	0.56
1:Q:13:MET:HG3	1:Y:19:LEU:HD11	1.86	0.56
2:E:444:LEU:HB2	3:E:66:DMF:H12	1.88	0.56
2:G:324:ASN:HB2	4:G:1736:HOH:O	2.04	0.56
1:Y:28:LYS:HB2	4:Y:1700:HOH:O	2.03	0.56
1:I:152:HIS:HB2	4:I:1601:HOH:O	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:173:GLU:CG	4:B:1646:HOH:O	2.29	0.55
2:J:348:THR:HG22	3:J:4:DMF:H22	1.88	0.55
1:Y:231:GLN:CA	4:Y:1576:HOH:O	2.48	0.55
1:O:105:GLN:NE2	4:O:1408:HOH:O	2.38	0.55
2:H:376:PHE:CD1	4:H:1358:HOH:O	2.50	0.55
2:X:362:GLU:HG3	4:X:1609:HOH:O	2.06	0.55
1:M:65:ALA:HA	4:M:1412:HOH:O	2.05	0.55
1:S:45:ASN:HA	4:S:1602:HOH:O	2.07	0.55
1:S:161:GLU:OE1	1:S:161:GLU:N	2.30	0.55
2:C:400:ALA:HB1	4:C:1253:HOH:O	2.06	0.55
2:H:409:ILE:HD11	4:H:1704:HOH:O	2.05	0.55
1:O:142:THR:HA	4:O:1391:HOH:O	2.06	0.54
2:H:301:OZT:H27	2:H:333:LYS:HE2	1.89	0.54
1:F:223:ARG:HD3	4:F:1550:HOH:O	2.05	0.54
2:C:515:ARG:HD2	4:C:1405:HOH:O	2.07	0.54
1:K:33:LEU:C	1:K:33:LEU:CD1	2.74	0.54
2:Z:456:GLN:HE21	2:Z:465:ARG:HH12	1.54	0.54
2:E:428:GLY:HA2	4:E:1096:HOH:O	2.08	0.54
1:Q:7:ILE:CG2	1:Q:8:SER:H	2.21	0.54
1:K:165:ASN:HA	4:K:1705:HOH:O	2.07	0.54
2:C:444:LEU:HB2	3:C:55:DMF:H13	1.88	0.54
1:A:167:LEU:O	1:A:171:TYR:HB2	2.08	0.54
1:D:9:PRO:HD3	1:Q:7:ILE:HD13	1.88	0.54
3:C:10:DMF:H12	4:C:1638:HOH:O	2.07	0.53
2:G:503:VAL:HA	4:G:1527:HOH:O	2.08	0.53
1:W:15:GLU:OE2	1:Y:9:PRO:HB3	2.08	0.53
1:M:33:LEU:HD12	1:M:33:LEU:C	2.28	0.53
2:L:456:GLN:HE21	2:L:465:ARG:HH22	1.55	0.53
1:Y:204:GLY:N	4:Y:1252:HOH:O	2.42	0.53
1:U:36:ALA:HA	1:U:174:ASN:OD1	2.08	0.53
2:T:451:LYS:NZ	2:X:473:ASP:OD1	2.41	0.53
1:F:203:LEU:N	4:F:1740:HOH:O	2.42	0.53
2:R:382:ARG:HH21	2:R:385:ILE:HD13	1.74	0.53
1:W:175:ALA:HB3	1:W:180:ALA:HB2	1.91	0.53
1:M:189:ARG:O	1:M:190:ALA:C	2.47	0.52
1:1:9:PRO:HB2	1:1:11:GLN:H	1.73	0.52
1:D:173:GLU:CA	1:D:174:ASN:HD22	2.18	0.52
1:Y:159:THR:HA	4:Y:1427:HOH:O	2.08	0.52
1:D:135:ARG:HB3	1:Q:48:ARG:HH22	1.75	0.52
2:E:444:LEU:H	3:E:66:DMF:H12	1.73	0.52
4:K:1762:HOH:O	1:M:135:ARG:HB3	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:456:GLN:NE2	2:V:465:ARG:NH2	2.53	0.51
4:K:1467:HOH:O	1:M:97:ARG:CD	2.45	0.51
1:M:97:ARG:NH1	4:M:1211:HOH:O	2.37	0.51
2:N:308:TYR:CZ	2:N:311:GLY:HA3	2.45	0.51
1:S:97:ARG:NH1	4:S:1727:HOH:O	2.36	0.51
1:I:105:GLN:NE2	4:I:1246:HOH:O	2.42	0.51
1:W:83:ASP:OD2	2:X:365:HIS:HD2	1.94	0.51
1:1:35:TYR:CZ	1:1:37:GLY:HA3	2.44	0.51
2:E:432:GLU:HG3	2:E:437:GLN:HB2	1.93	0.51
2:J:391:LEU:O	2:J:392:ALA:HB2	2.10	0.51
1:K:59:ARG:HB2	4:K:1392:HOH:O	2.10	0.51
3:N:22:DMF:C1	4:P:1377:HOH:O	2.58	0.51
1:F:136:PRO:HG3	4:F:1598:HOH:O	2.10	0.51
1:Y:9:PRO:HB2	1:Y:11:GLN:H	1.75	0.51
1:M:76:ARG:HD3	4:M:647:HOH:O	2.09	0.51
2:2:456:GLN:HE22	2:2:465:ARG:NH2	2.04	0.51
1:D:13:MET:HG3	1:Q:19:LEU:HD11	1.93	0.51
1:M:40:LEU:HD13	1:M:212:VAL:CG1	2.41	0.51
1:1:67:LYS:HE3	1:1:69:ASN:HD21	1.76	0.50
2:J:411:ALA:HB1	4:J:1667:HOH:O	2.11	0.50
1:Q:8:SER:H	1:Q:11:GLN:HB3	1.77	0.50
1:I:205:VAL:HG21	1:I:231:GLN:HG2	1.94	0.50
2:Z:307:LYS:HD3	4:Z:277:HOH:O	2.11	0.50
2:R:348:THR:HG23	4:R:1446:HOH:O	2.11	0.50
1:W:175:ALA:CB	1:W:180:ALA:HB2	2.41	0.50
2:C:445:PHE:CD2	3:C:55:DMF:C1	2.95	0.50
1:Q:76:ARG:HD3	4:Q:411:HOH:O	2.12	0.50
2:Z:456:GLN:HE21	2:Z:465:ARG:NH1	2.08	0.50
1:W:231:GLN:CA	4:W:1447:HOH:O	2.51	0.50
2:L:317:ASP:OD1	2:L:333:LYS:NZ	2.44	0.50
1:F:135:ARG:NH1	4:F:1640:HOH:O	2.44	0.50
2:Z:515:ARG:HD2	4:Z:1691:HOH:O	2.12	0.50
1:D:173:GLU:CB	1:D:174:ASN:HD22	2.21	0.49
1:M:40:LEU:CD1	1:M:212:VAL:CG1	2.90	0.49
2:L:391:LEU:HD12	2:L:399:LEU:HD23	1.92	0.49
1:U:69:ASN:N	1:U:69:ASN:ND2	2.59	0.49
1:S:35:TYR:CZ	1:S:37:GLY:HA3	2.47	0.49
1:M:223:ARG:CD	4:M:1631:HOH:O	2.60	0.49
2:V:409:ILE:CG2	4:V:1453:HOH:O	2.60	0.49
1:A:105:GLN:NE2	4:A:1308:HOH:O	2.45	0.49
2:R:362:GLU:OE2	2:R:382:ARG:HD3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:41:PHE:CD1	1:W:63:ALA:HB2	2.48	0.49
1:F:105:GLN:NE2	4:F:1457:HOH:O	2.46	0.49
1:S:97:ARG:N	4:S:1484:HOH:O	2.34	0.49
1:Q:48:ARG:HB3	4:Q:1636:HOH:O	2.12	0.49
1:1:67:LYS:HG2	1:1:69:ASN:ND2	2.27	0.49
1:D:173:GLU:CB	1:D:174:ASN:HD21	2.19	0.49
1:A:223:ARG:HD2	4:A:1724:HOH:O	2.12	0.49
1:O:204:GLY:N	4:O:1277:HOH:O	2.45	0.48
2:2:465:ARG:HG3	2:2:513:LEU:HD22	1.94	0.48
1:O:56:LEU:HG	1:O:62:PHE:HB2	1.94	0.48
2:T:432:GLU:O	4:T:1228:HOH:O	2.20	0.48
1:Y:56:LEU:HG	1:Y:62:PHE:HB2	1.96	0.48
1:A:90:ASP:OD1	1:A:93:ASP:N	2.46	0.48
1:U:54:SER:CB	1:U:75:ARG:HD2	2.43	0.48
2:X:320:SER:HB3	2:X:331:VAL:HG21	1.95	0.48
1:U:163:ILE:HG23	1:U:187:ALA:O	2.13	0.48
2:V:390:ASN:HD22	2:V:390:ASN:N	2.11	0.48
1:I:56:LEU:HG	1:I:62:PHE:HB2	1.94	0.48
2:R:465:ARG:HD3	4:R:1108:HOH:O	2.14	0.48
2:G:476:ASP:OD1	3:G:12:DMF:H12	2.13	0.48
1:S:171:TYR:HE2	1:S:173:GLU:HG2	1.78	0.48
1:M:51:GLN:NE2	1:M:75:ARG:CZ	2.77	0.48
1:O:97:ARG:HH11	1:O:97:ARG:HG2	1.78	0.48
1:M:182:ARG:CB	4:M:1510:HOH:O	2.46	0.48
1:M:102:VAL:HG12	3:M:249:DMF:H22	1.95	0.48
1:A:13:MET:HG3	1:O:19:LEU:HD11	1.94	0.48
1:B:209:GLU:HB2	4:B:1563:HOH:O	2.12	0.48
1:Q:51:GLN:HB2	4:Q:851:HOH:O	2.14	0.48
1:1:189:ARG:HH11	1:1:203:LEU:HB2	1.79	0.48
1:K:51:GLN:NE2	1:K:75:ARG:CZ	2.77	0.48
1:D:9:PRO:N	4:D:1284:HOH:O	2.46	0.48
1:1:33:LEU:O	1:1:33:LEU:HD12	2.14	0.48
1:W:230:LEU:C	4:W:1447:HOH:O	2.52	0.48
2:C:444:LEU:HB2	3:C:55:DMF:C1	2.44	0.48
1:B:56:LEU:HG	1:B:62:PHE:HB2	1.96	0.48
2:V:376:PHE:CE2	2:V:380:ILE:HD11	2.49	0.48
1:O:10:GLU:HB2	4:O:1774:HOH:O	2.12	0.47
1:M:51:GLN:HE21	1:M:75:ARG:CZ	2.26	0.47
1:Q:56:LEU:HG	1:Q:62:PHE:HB2	1.96	0.47
1:1:30:VAL:HG13	1:1:43:ALA:HB2	1.96	0.47
1:Y:163:ILE:HG23	1:Y:187:ALA:O	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:456:GLN:HE22	2:R:465:ARG:NH2	2.11	0.47
2:N:464:LEU:HD21	2:N:505:VAL:HG11	1.96	0.47
2:N:415:GLN:NE2	4:N:541:HOH:O	2.47	0.47
1:S:65:ALA:HA	4:S:1382:HOH:O	2.14	0.47
1:1:41:PHE:CE1	1:1:63:ALA:HB2	2.49	0.47
1:U:92:ARG:NE	4:U:1709:HOH:O	2.46	0.47
2:R:465:ARG:HG3	2:R:513:LEU:HD22	1.96	0.47
1:B:209:GLU:HG3	4:B:1563:HOH:O	2.13	0.47
1:M:56:LEU:HG	1:M:62:PHE:HB2	1.97	0.47
1:O:51:GLN:HE21	1:O:75:ARG:CZ	2.28	0.47
2:Z:515:ARG:CD	4:Z:1691:HOH:O	2.63	0.47
3:M:249:DMF:H12	4:M:1743:HOH:O	2.15	0.47
2:P:301:OZT:H27	2:P:333:LYS:HE2	1.95	0.47
2:J:320:SER:HB3	2:J:331:VAL:HG21	1.95	0.47
2:N:306:LEU:HD12	2:N:306:LEU:C	2.35	0.47
1:Y:234:LEU:CD2	1:Y:234:LEU:C	2.78	0.47
2:E:456:GLN:HE21	2:E:465:ARG:HH12	1.62	0.47
1:I:30:VAL:HG13	1:I:43:ALA:HB2	1.96	0.47
2:V:428:GLY:HA2	4:V:1440:HOH:O	2.14	0.47
1:S:56:LEU:HG	1:S:62:PHE:HB2	1.95	0.47
1:Y:231:GLN:C	4:Y:1576:HOH:O	2.53	0.47
1:K:56:LEU:HG	1:K:62:PHE:HB2	1.96	0.47
3:J:4:DMF:H23	4:J:1466:HOH:O	2.07	0.46
1:W:56:LEU:HG	1:W:62:PHE:HB2	1.97	0.46
3:T:29:DMF:C2	4:T:1567:HOH:O	2.55	0.46
1:S:97:ARG:HB2	4:S:1727:HOH:O	2.05	0.46
1:A:56:LEU:HG	1:A:62:PHE:HB2	1.96	0.46
2:L:331:VAL:HG13	2:L:349:ALA:HB2	1.98	0.46
2:P:483:GLY:HA2	4:P:38:HOH:O	2.14	0.46
1:K:33:LEU:HD12	1:K:40:LEU:HB3	1.96	0.46
2:H:332:ARG:CD	4:H:1570:HOH:O	2.41	0.46
1:F:22:LYS:HE2	4:F:1400:HOH:O	2.15	0.46
3:L:53:DMF:HC	4:L:1603:HOH:O	2.14	0.46
1:W:205:VAL:CG2	4:W:1447:HOH:O	2.63	0.46
2:E:377:ALA:HB1	3:L:53:DMF:HC	1.98	0.46
2:N:301:OZT:H27	2:N:333:LYS:HE2	1.97	0.46
1:Y:159:THR:CA	4:Y:1427:HOH:O	2.63	0.46
1:D:217:ARG:NH1	4:D:1496:HOH:O	2.44	0.46
1:D:30:VAL:HG13	1:D:43:ALA:HB2	1.98	0.46
1:K:51:GLN:HG2	4:K:561:HOH:O	2.15	0.46
1:B:67:LYS:HG2	1:B:69:ASN:HD21	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:430:ASN:HB2	4:J:1239:HOH:O	2.15	0.45
4:M:1478:HOH:O	2:N:361:VAL:HG22	2.06	0.45
1:U:35:TYR:CD1	1:U:36:ALA:N	2.84	0.45
1:K:51:GLN:HE21	1:K:75:ARG:CZ	2.29	0.45
1:Q:16:ARG:NH1	1:Q:117:PRO:HD3	2.31	0.45
1:A:152:HIS:CB	1:A:171:TYR:HE2	2.25	0.45
2:Z:331:VAL:HG13	2:Z:349:ALA:HB2	1.98	0.45
1:U:56:LEU:HG	1:U:62:PHE:HB2	1.97	0.45
1:B:30:VAL:HG13	1:B:43:ALA:HB2	1.97	0.45
1:Y:83:ASP:OD2	2:Z:365:HIS:HD2	1.99	0.45
1:W:231:GLN:N	4:W:1447:HOH:O	2.50	0.45
1:M:40:LEU:CD1	1:M:212:VAL:HG12	2.47	0.45
2:C:301:OZT:H27	2:C:333:LYS:HE2	1.97	0.45
2:L:509:ARG:HD3	4:L:1362:HOH:O	2.16	0.45
1:1:56:LEU:HG	1:1:62:PHE:HB2	1.99	0.45
2:H:509:ARG:HD3	4:H:1309:HOH:O	2.17	0.45
1:A:83:ASP:OD2	2:H:365:HIS:HD2	2.00	0.45
1:D:182:ARG:HD3	4:D:1270:HOH:O	2.17	0.45
1:D:9:PRO:CD	1:Q:7:ILE:CD1	2.95	0.45
1:O:87:TYR:O	2:P:357:ARG:NH2	2.49	0.45
1:Y:171:TYR:CE1	4:Y:1692:HOH:O	2.56	0.45
1:1:36:ALA:HB2	1:1:174:ASN:O	2.16	0.45
2:T:515:ARG:HD2	4:T:1505:HOH:O	2.15	0.45
2:G:320:SER:HB3	2:G:331:VAL:HG21	1.99	0.45
1:I:76:ARG:HD3	4:I:977:HOH:O	2.17	0.45
1:M:30:VAL:HG13	1:M:43:ALA:HB2	1.99	0.45
1:S:146:SER:HA	4:S:1501:HOH:O	2.17	0.45
1:M:92:ARG:CG	1:M:92:ARG:O	2.64	0.44
1:D:135:ARG:HB3	1:Q:48:ARG:NH2	2.32	0.44
1:O:51:GLN:NE2	1:O:75:ARG:CZ	2.80	0.44
1:Y:30:VAL:HG13	1:Y:43:ALA:HB2	1.99	0.44
1:Q:85:ARG:HD3	4:Q:1588:HOH:O	2.16	0.44
1:A:30:VAL:HG13	1:A:43:ALA:HB2	1.99	0.44
1:K:32:ALA:HA	1:K:40:LEU:O	2.16	0.44
2:R:430:ASN:ND2	4:R:1315:HOH:O	2.50	0.44
3:G:12:DMF:H13	4:V:1271:HOH:O	2.17	0.44
1:M:129:HIS:NE2	4:M:1739:HOH:O	2.35	0.44
1:Y:35:TYR:HD2	1:Y:38:GLY:O	1.96	0.44
1:U:11:GLN:CG	4:U:1729:HOH:O	2.57	0.44
1:B:67:LYS:HG2	1:B:69:ASN:ND2	2.33	0.44
2:X:301:OZT:O	2:X:440:GLY:HA3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:54:SER:HB2	4:S:1464:HOH:O	2.16	0.44
2:T:422:SER:OG	2:T:432:GLU:OE2	2.30	0.44
1:D:56:LEU:HG	1:D:62:PHE:HB2	2.00	0.44
1:A:67:LYS:HG2	1:A:69:ASN:HD21	1.83	0.44
1:Y:35:TYR:CE1	1:Y:37:GLY:CA	3.00	0.44
2:C:301:OZT:O	2:C:440:GLY:HA3	2.17	0.44
1:U:30:VAL:HG13	1:U:43:ALA:HB2	1.99	0.44
2:X:401:LEU:HD12	4:X:1614:HOH:O	2.18	0.44
1:M:40:LEU:HD13	1:M:212:VAL:HG12	2.00	0.44
2:E:456:GLN:NE2	2:E:465:ARG:NH1	2.65	0.43
1:F:22:LYS:CE	4:F:1400:HOH:O	2.66	0.43
1:Q:162:PRO:HA	4:Q:1424:HOH:O	2.18	0.43
1:W:223:ARG:HA	4:W:1590:HOH:O	2.17	0.43
2:R:320:SER:HB3	2:R:331:VAL:HG21	2.00	0.43
1:B:16:ARG:NH1	1:B:117:PRO:HD3	2.33	0.43
1:S:30:VAL:HG13	1:S:43:ALA:HB2	1.98	0.43
2:2:401:LEU:HA	2:2:402:PRO:HD3	1.88	0.43
1:M:65:ALA:CA	4:M:1412:HOH:O	2.64	0.43
1:F:67:LYS:HG2	1:F:69:ASN:HD21	1.84	0.43
1:M:114:GLN:NE2	4:M:1597:HOH:O	2.52	0.43
1:Y:35:TYR:CE1	1:Y:37:GLY:N	2.82	0.43
1:S:74:LEU:HD13	1:S:122:LEU:HD11	2.01	0.43
2:R:356:ALA:CB	3:R:34:DMF:H22	2.49	0.43
2:R:357:ARG:O	2:R:361:VAL:HG23	2.19	0.43
2:C:376:PHE:HD1	4:C:1247:HOH:O	2.02	0.43
2:E:320:SER:HB3	2:E:331:VAL:HG21	2.01	0.43
2:V:422:SER:OG	2:V:432:GLU:OE2	2.29	0.42
1:Y:84:THR:CG2	4:Y:1479:HOH:O	2.67	0.42
1:W:140:ARG:NH2	4:W:1077:HOH:O	2.45	0.42
1:K:30:VAL:HG13	1:K:43:ALA:HB2	2.01	0.42
4:E:1508:HOH:O	1:K:90:ASP:HB2	2.19	0.42
1:O:35:TYR:HE1	4:O:1616:HOH:O	2.02	0.42
2:J:415:GLN:CB	4:J:1632:HOH:O	2.66	0.42
1:F:30:VAL:HG13	1:F:43:ALA:HB2	2.00	0.42
3:K:250:DMF:C	4:K:1485:HOH:O	2.67	0.42
2:T:301:OZT:O	2:T:440:GLY:HA3	2.18	0.42
2:Z:301:OZT:O	2:Z:440:GLY:HA3	2.20	0.42
2:T:432:GLU:HG3	2:T:437:GLN:HB2	2.01	0.42
1:A:67:LYS:HG2	1:A:69:ASN:ND2	2.35	0.42
2:V:391:LEU:O	2:V:392:ALA:HB2	2.19	0.42
1:D:205:VAL:HG13	1:D:230:LEU:HD23	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:457:VAL:HA	2:E:462:SER:HB3	2.02	0.42
2:T:320:SER:HB3	2:T:331:VAL:HG21	2.00	0.42
1:Q:69:ASN:HD22	1:Q:69:ASN:H	1.68	0.42
1:Q:31:VAL:HG12	1:Q:155:VAL:HG22	2.02	0.42
1:W:31:VAL:HG12	1:W:155:VAL:HG22	2.02	0.42
1:F:161:GLU:N	1:F:161:GLU:CD	2.72	0.42
2:V:301:OZT:C7	2:V:333:LYS:HE2	2.50	0.42
1:F:87:TYR:O	2:G:357:ARG:NH2	2.53	0.42
1:Q:28:LYS:CE	4:Q:1387:HOH:O	2.62	0.42
1:1:174:ASN:O	1:1:175:ALA:C	2.58	0.42
2:Z:301:OZT:H27	2:Z:333:LYS:HE2	2.01	0.42
1:W:205:VAL:HG22	4:W:1447:HOH:O	2.19	0.42
1:Q:217:ARG:NH2	4:Q:1650:HOH:O	2.52	0.42
2:E:364:GLU:HB3	4:E:1451:HOH:O	2.18	0.42
1:D:173:GLU:CA	1:D:174:ASN:ND2	2.82	0.42
4:K:1467:HOH:O	1:M:97:ARG:NE	2.52	0.42
1:A:69:ASN:H	1:A:69:ASN:HD22	1.68	0.42
2:Z:444:LEU:HD12	4:Z:1433:HOH:O	2.20	0.42
1:F:129:HIS:CD2	4:F:1726:HOH:O	2.73	0.42
2:V:437:GLN:HG3	2:V:438:ALA:N	2.35	0.42
2:E:444:LEU:HD13	3:E:66:DMF:H23	2.02	0.42
1:D:97:ARG:HD2	1:Q:49:SER:O	2.20	0.42
2:2:456:GLN:NE2	2:2:465:ARG:HH12	2.16	0.41
1:A:217:ARG:HA	1:A:218:PRO:HD3	1.85	0.41
1:A:223:ARG:CD	4:A:1724:HOH:O	2.68	0.41
1:U:189:ARG:O	1:U:190:ALA:C	2.58	0.41
2:J:362:GLU:OE2	2:J:382:ARG:HD3	2.20	0.41
2:Z:476:ASP:OD1	3:Z:18:DMF:H22	2.20	0.41
1:B:69:ASN:HD22	1:B:69:ASN:H	1.68	0.41
2:T:464:LEU:HD21	2:T:505:VAL:HG11	2.01	0.41
1:Q:30:VAL:HG13	1:Q:43:ALA:HB2	2.02	0.41
1:F:69:ASN:H	1:F:69:ASN:HD22	1.68	0.41
2:P:320:SER:HB3	2:P:331:VAL:HG21	2.02	0.41
1:Q:181:LEU:O	1:Q:185:VAL:HG23	2.20	0.41
2:X:444:LEU:HD13	4:X:1671:HOH:O	2.21	0.41
1:1:14:ARG:HG2	4:1:1788:HOH:O	2.07	0.41
1:S:51:GLN:HB2	4:S:1464:HOH:O	2.20	0.41
1:B:31:VAL:HG12	1:B:155:VAL:HG22	2.02	0.41
1:U:42:VAL:HG12	1:U:188:LEU:HD21	2.02	0.41
1:W:67:LYS:HG2	1:W:69:ASN:HD21	1.86	0.41
1:D:88:ALA:HB2	4:D:535:HOH:O	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:391:LEU:HD12	2:R:399:LEU:HD23	2.03	0.41
1:M:67:LYS:HG2	1:M:69:ASN:HD21	1.84	0.41
2:R:332:ARG:NE	4:R:1547:HOH:O	2.35	0.41
2:R:361:VAL:O	2:R:365:HIS:HB2	2.21	0.41
1:M:92:ARG:HG3	1:M:92:ARG:O	2.20	0.41
2:P:388:ARG:NH1	4:P:1095:HOH:O	2.53	0.41
1:K:189:ARG:CD	4:K:1741:HOH:O	2.32	0.41
1:D:22:LYS:NZ	1:K:10:GLU:OE1	2.54	0.41
2:E:483:GLY:HA2	4:E:1046:HOH:O	2.20	0.41
2:L:301:OZT:O	2:L:440:GLY:HA3	2.20	0.41
1:D:161:GLU:HB2	1:D:162:PRO:HD3	2.03	0.41
2:X:401:LEU:HA	2:X:402:PRO:HD3	1.82	0.41
1:S:67:LYS:HG2	1:S:69:ASN:HD21	1.86	0.41
2:G:444:LEU:HD21	2:X:325:MET:SD	2.61	0.41
1:S:35:TYR:CE1	1:S:37:GLY:CA	3.02	0.41
2:N:301:OZT:O	2:N:440:GLY:HA3	2.21	0.41
1:F:67:LYS:HG2	1:F:69:ASN:ND2	2.35	0.41
1:M:47:SER:HA	4:M:1402:HOH:O	2.20	0.41
1:K:150:GLU:HA	1:K:151:PRO:HD3	1.95	0.41
1:W:30:VAL:HG13	1:W:43:ALA:HB2	2.02	0.41
1:D:67:LYS:HG2	1:D:69:ASN:HD21	1.86	0.41
2:V:335:TYR:HB3	3:V:27:DMF:H12	2.01	0.41
1:D:31:VAL:HG12	1:D:155:VAL:HG22	2.02	0.41
1:D:83:ASP:OD2	2:E:365:HIS:HD2	2.03	0.41
1:Q:67:LYS:HG2	1:Q:69:ASN:HD21	1.87	0.40
1:M:67:LYS:HG2	1:M:69:ASN:ND2	2.35	0.40
2:H:479:SER:HB2	2:L:479:SER:HB2	2.02	0.40
1:I:67:LYS:HG2	1:I:69:ASN:HD21	1.86	0.40
2:V:390:ASN:H	2:V:390:ASN:HD22	1.70	0.40
1:O:51:GLN:NE2	4:O:937:HOH:O	2.54	0.40
2:P:483:GLY:HA3	3:P:14:DMF:H11	2.03	0.40
1:F:45:ASN:HA	1:F:46:PRO:HD2	2.01	0.40
1:Y:67:LYS:HE3	1:Y:69:ASN:HD21	1.85	0.40
2:H:301:OZT:O	2:H:440:GLY:HA3	2.22	0.40
2:P:301:OZT:O	2:P:440:GLY:HA3	2.22	0.40
1:W:31:VAL:HG23	1:W:42:VAL:HB	2.02	0.40
2:G:350:ALA:CB	4:G:1411:HOH:O	2.69	0.40
1:I:214:ASP:O	1:I:217:ARG:HG3	2.22	0.40
1:O:67:LYS:HG2	1:O:69:ASN:ND2	2.37	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

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

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

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1	164/192 (85%)	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

All (115) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	69	ASN
1	A	159	THR
1	A	173	GLU
1	A	188	LEU
1	A	234	LEU
1	B	69	ASN
1	B	113	GLU
1	B	159	THR
2	C	322	GLN
2	C	345	ILE
2	C	444	LEU
2	C	497	ILE
2	C	509	ARG
1	D	69	ASN
1	D	159	THR
1	D	174	ASN
2	E	317	ASP
2	E	330	ASP
2	E	345	ILE
2	E	401	LEU
2	E	462	SER
1	F	69	ASN
1	F	159	THR

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Mol	Chain	Res	Type
2	G	338	ASP
2	G	345	ILE
2	G	444	LEU
2	G	465	ARG
2	G	492	PRO
2	H	330	ASP
2	H	338	ASP
2	H	345	ILE
2	H	386	MET
2	H	391	LEU
2	H	444	LEU
1	I	33	LEU
1	I	69	ASN
1	I	159	THR
1	I	160	THR
1	I	174	ASN
1	I	233	LEU
2	J	345	ILE
1	K	33	LEU
1	K	69	ASN
1	K	113	GLU
1	K	159	THR
1	K	234	LEU
2	L	338	ASP
2	L	345	ILE
2	L	444	LEU
2	L	519	GLU
1	M	69	ASN
1	M	159	THR
1	M	181	LEU
1	M	188	LEU
2	N	322	GLN
2	N	338	ASP
2	N	345	ILE
2	N	461	ASP
2	N	465	ARG
1	O	69	ASN
1	O	98	GLN
1	O	99	LEU
1	O	109	THR
1	O	159	THR
2	P	322	GLN

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Mol	Chain	Res	Type
2	P	345	ILE
2	P	433	GLU
1	Q	9	PRO
1	Q	69	ASN
1	Q	159	THR
1	Q	169	GLU
1	Q	203	LEU
1	Q	234	LEU
2	R	322	GLN
2	R	338	ASP
2	R	345	ILE
2	R	362	GLU
2	R	382	ARG
2	R	515	ARG
1	S	69	ASN
1	S	159	THR
1	S	217	ARG
2	T	345	ILE
2	T	444	LEU
1	U	8	SER
1	U	35	TYR
1	U	69	ASN
1	U	113	GLU
1	U	159	THR
1	U	169	GLU
1	U	173	GLU
1	U	188	LEU
2	V	322	GLN
2	V	345	ILE
2	V	503	VAL
1	W	69	ASN
1	W	113	GLU
1	W	159	THR
1	W	176	SER
1	W	203	LEU
2	X	338	ASP
2	X	345	ILE
1	Y	69	ASN
1	Y	113	GLU
1	Y	159	THR
1	Y	234	LEU
2	Z	338	ASP

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Mol	Chain	Res	Type
2	Z	345	ILE
2	Z	477	ASP
1	1	33	LEU
1	1	69	ASN
1	1	159	THR
2	2	322	GLN
2	2	345	ILE
2	2	462	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (66) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	69	ASN
1	A	114	GLN
1	A	129	HIS
1	B	69	ASN
1	B	114	GLN
1	B	129	HIS
2	C	365	HIS
2	C	456	GLN
1	D	69	ASN
1	D	114	GLN
1	D	129	HIS
1	D	174	ASN
2	E	365	HIS
2	E	456	GLN
1	F	69	ASN
1	F	231	GLN
2	G	365	HIS
2	G	456	GLN
2	H	365	HIS
2	H	456	GLN
1	I	69	ASN
1	I	231	GLN
2	J	365	HIS
2	J	456	GLN
1	K	51	GLN
1	K	69	ASN
1	K	129	HIS
2	L	365	HIS
2	L	456	GLN
1	M	51	GLN

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Mol	Chain	Res	Type
1	M	69	ASN
2	N	365	HIS
2	N	415	GLN
2	N	456	GLN
1	O	51	GLN
1	O	69	ASN
1	O	98	GLN
1	O	105	GLN
1	O	152	HIS
2	P	365	HIS
2	P	456	GLN
1	Q	69	ASN
2	R	365	HIS
2	R	456	GLN
1	S	69	ASN
1	S	114	GLN
2	T	365	HIS
2	T	456	GLN
1	U	69	ASN
1	U	216	ASN
2	V	365	HIS
2	V	390	ASN
2	V	437	GLN
2	V	456	GLN
1	W	69	ASN
1	W	114	GLN
1	W	129	HIS
2	X	365	HIS
2	X	456	GLN
1	Y	69	ASN
2	Z	365	HIS
2	Z	456	GLN
1	1	69	ASN
1	1	114	GLN
2	2	365	HIS
2	2	456	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

14 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	OZT	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

All (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
2	E	301	OZT	C2-CA	-3.29	1.47	1.54
2	2	301	OZT	C2-CA	-3.24	1.47	1.54
2	G	301	OZT	C2-CA	-3.15	1.47	1.54
2	V	301	OZT	C2-CA	-3.09	1.47	1.54
2	X	301	OZT	O1-C2	-2.97	1.41	1.46
2	H	301	OZT	O1-C2	-2.96	1.41	1.46
2	L	301	OZT	C2-CA	-2.89	1.48	1.54
2	L	301	OZT	O1-C2	-2.88	1.42	1.46
2	V	301	OZT	O1-C2	-2.85	1.42	1.46
2	2	301	OZT	O1-C2	-2.81	1.42	1.46
2	C	301	OZT	C2-CA	-2.81	1.48	1.54
2	J	301	OZT	C2-CA	-2.78	1.48	1.54
2	J	301	OZT	O1-C2	-2.77	1.42	1.46
2	C	301	OZT	O1-C2	-2.76	1.42	1.46
2	R	301	OZT	O1-C2	-2.75	1.42	1.46
2	E	301	OZT	O1-C2	-2.73	1.42	1.46
2	Z	301	OZT	O1-C2	-2.64	1.42	1.46
2	T	301	OZT	O1-C2	-2.57	1.42	1.46
2	T	301	OZT	C2-CA	-2.50	1.49	1.54
2	N	301	OZT	O1-C2	-2.47	1.42	1.46
2	N	301	OZT	C2-CA	-2.47	1.49	1.54
2	P	301	OZT	O1-C2	-2.07	1.43	1.46
2	X	301	OZT	C5-N	2.40	1.37	1.33
2	H	301	OZT	C5-N	2.90	1.38	1.33
2	E	301	OZT	C5-N	3.29	1.38	1.33
2	2	301	OZT	C5-N	3.34	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	301	OZT	C5-N	3.41	1.38	1.33
2	P	301	OZT	C5-N	3.42	1.38	1.33
2	T	301	OZT	C5-N	3.55	1.38	1.33
2	L	301	OZT	C5-N	3.62	1.39	1.33
2	C	301	OZT	C5-N	3.70	1.39	1.33
2	G	301	OZT	C5-N	3.73	1.39	1.33
2	R	301	OZT	C5-N	3.82	1.39	1.33
2	N	301	OZT	C5-N	3.86	1.39	1.33
2	Z	301	OZT	C5-N	4.29	1.40	1.33
2	V	301	OZT	C5-N	4.68	1.40	1.33
2	V	301	OZT	O1-C5	8.66	1.47	1.36
2	2	301	OZT	O1-C5	8.70	1.47	1.36
2	Z	301	OZT	O1-C5	8.79	1.48	1.36
2	N	301	OZT	O1-C5	9.03	1.48	1.36
2	P	301	OZT	O1-C5	9.03	1.48	1.36
2	G	301	OZT	O1-C5	9.07	1.48	1.36
2	X	301	OZT	O1-C5	9.22	1.48	1.36
2	H	301	OZT	O1-C5	9.37	1.48	1.36
2	T	301	OZT	O1-C5	9.39	1.48	1.36
2	J	301	OZT	O1-C5	9.57	1.49	1.36
2	L	301	OZT	O1-C5	9.82	1.49	1.36
2	R	301	OZT	O1-C5	9.94	1.49	1.36
2	C	301	OZT	O1-C5	9.97	1.49	1.36
2	E	301	OZT	O1-C5	10.16	1.49	1.36

All (67) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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
2	2	301	OZT	O6-C5-N	-6.93	120.74	129.16
2	G	301	OZT	O6-C5-N	-6.77	120.94	129.16
2	C	301	OZT	O6-C5-N	-6.72	121.00	129.16
2	N	301	OZT	O6-C5-N	-6.71	121.00	129.16
2	P	301	OZT	O6-C5-N	-6.67	121.06	129.16
2	E	301	OZT	O6-C5-N	-6.57	121.18	129.16
2	Z	301	OZT	O6-C5-N	-6.53	121.23	129.16
2	R	301	OZT	O6-C5-N	-6.34	121.46	129.16
2	V	301	OZT	O6-C5-N	-6.25	121.57	129.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	V	301	OZT	C7-C2-CA	-4.64	108.19	114.67
2	H	301	OZT	C7-C2-CA	-4.37	108.57	114.67
2	P	301	OZT	C7-C2-CA	-4.21	108.79	114.67
2	N	301	OZT	C7-C2-CA	-4.13	108.91	114.67
2	G	301	OZT	C7-C2-CA	-4.12	108.92	114.67
2	Z	301	OZT	C7-C2-CA	-4.10	108.94	114.67
2	T	301	OZT	C7-C2-CA	-4.07	108.99	114.67
2	R	301	OZT	C7-C2-CA	-4.06	109.00	114.67
2	L	301	OZT	C7-C2-CA	-4.05	109.02	114.67
2	J	301	OZT	C7-C2-CA	-4.00	109.08	114.67
2	C	301	OZT	C7-C2-CA	-3.95	109.16	114.67
2	X	301	OZT	C7-C2-CA	-3.93	109.19	114.67
2	E	301	OZT	C7-C2-CA	-3.86	109.29	114.67
2	2	301	OZT	C7-C2-CA	-3.83	109.32	114.67
2	R	301	OZT	O-C-CA	-2.47	118.17	125.74
2	G	301	OZT	O-C-CA	-2.27	118.78	125.74
2	V	301	OZT	O-C-CA	-2.23	118.89	125.74
2	L	301	OZT	O-C-CA	-2.20	118.99	125.74
2	T	301	OZT	O-C-CA	-2.19	119.01	125.74
2	C	301	OZT	O-C-CA	-2.17	119.07	125.74
2	E	301	OZT	O-C-CA	-2.16	119.11	125.74
2	N	301	OZT	O-C-CA	-2.16	119.11	125.74
2	P	301	OZT	O-C-CA	-2.13	119.20	125.74
2	2	301	OZT	O-C-CA	-2.10	119.29	125.74
2	J	301	OZT	O-C-CA	-2.01	119.56	125.74
2	X	301	OZT	O1-C2-CA	2.91	108.02	103.42
2	E	301	OZT	O1-C2-CA	3.19	108.46	103.42
2	R	301	OZT	O1-C2-CA	3.30	108.62	103.42
2	2	301	OZT	O1-C2-CA	3.41	108.80	103.42
2	H	301	OZT	O1-C2-CA	3.44	108.84	103.42
2	Z	301	OZT	O1-C2-CA	3.44	108.84	103.42
2	T	301	OZT	O1-C2-CA	3.46	108.87	103.42
2	J	301	OZT	O1-C2-CA	3.48	108.91	103.42
2	G	301	OZT	O1-C2-CA	3.51	108.95	103.42
2	L	301	OZT	O1-C2-CA	3.51	108.96	103.42
2	C	301	OZT	O1-C2-CA	3.53	108.99	103.42
2	N	301	OZT	O1-C2-CA	3.66	109.19	103.42
2	P	301	OZT	O1-C2-CA	3.75	109.33	103.42
2	V	301	OZT	O1-C2-CA	4.82	111.02	103.42
2	E	301	OZT	O1-C5-N	7.34	116.94	109.84
2	R	301	OZT	O1-C5-N	7.46	117.05	109.84
2	G	301	OZT	O1-C5-N	7.81	117.39	109.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	301	OZT	O1-C5-N	7.91	117.49	109.84
2	X	301	OZT	O1-C5-N	7.96	117.53	109.84
2	Z	301	OZT	O1-C5-N	8.01	117.58	109.84
2	H	301	OZT	O1-C5-N	8.01	117.58	109.84
2	V	301	OZT	O1-C5-N	8.08	117.65	109.84
2	P	301	OZT	O1-C5-N	8.18	117.74	109.84
2	N	301	OZT	O1-C5-N	8.19	117.75	109.84
2	L	301	OZT	O1-C5-N	8.20	117.76	109.84
2	2	301	OZT	O1-C5-N	8.20	117.77	109.84
2	J	301	OZT	O1-C5-N	8.29	117.86	109.84
2	T	301	OZT	O1-C5-N	8.47	118.03	109.84

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 (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

67 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length

(or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	DMF	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
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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	Z	18	DMF	2	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	1	215/248 (86%)	0.54	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

All (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
1	U	204	GLY	6.0
1	W	7	ILE	5.9
1	Y	10	GLU	5.9
1	W	161	GLU	5.7
1	Q	7	ILE	5.5
1	Y	9	PRO	5.4
1	Y	184	ALA	5.4
1	A	11	GLN	5.4
1	Y	131	GLY	5.1
1	U	206	ALA	5.0
1	Y	11	GLN	4.9
1	D	12	ALA	4.8
1	I	203	LEU	4.8
1	A	169	GLU	4.7
1	Y	14	ARG	4.7
1	A	191	GLY	4.7
1	Y	188	LEU	4.7
1	Q	169	GLU	4.7
1	Y	13	MET	4.6
1	U	205	VAL	4.6
1	O	161	GLU	4.6
1	Y	179	ASP	4.5
1	D	182	ARG	4.5
1	S	172	ALA	4.5
1	F	11	GLN	4.3
1	U	48	ARG	4.3
1	M	206	ALA	4.3

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Mol	Chain	Res	Type	RSRZ
1	A	48	ARG	4.2
1	Y	169	GLU	4.2
1	Y	133	THR	4.2
1	S	188	LEU	4.1
1	M	172	ALA	4.1
1	M	9	PRO	4.1
1	K	11	GLN	4.1
1	U	231	GLN	4.1
1	W	14	ARG	4.1
1	M	8	SER	4.0
1	I	205	VAL	4.0
2	R	412	SER	4.0
1	S	169	GLU	4.0
1	F	48	ARG	4.0
1	Q	10	GLU	3.9
1	M	12	ALA	3.9
1	O	8	SER	3.9
1	K	233	LEU	3.9
1	K	203	LEU	3.8
1	M	113	GLU	3.8
1	W	160	THR	3.8
1	K	10	GLU	3.8
1	B	231	GLN	3.7
1	S	36	ALA	3.7
1	O	172	ALA	3.7
1	B	48	ARG	3.7
1	K	179	ASP	3.7
1	D	131	GLY	3.7
1	Y	171	TYR	3.7
1	D	188	LEU	3.7
1	1	234	LEU	3.7
1	U	10	GLU	3.6
1	D	14	ARG	3.6
1	S	173	GLU	3.6
1	A	135	ARG	3.6
1	S	182	ARG	3.6
1	B	232	ALA	3.6
1	S	232	ALA	3.6
1	B	227	GLY	3.6
1	I	188	LEU	3.6
1	K	169	GLU	3.5
1	S	48	ARG	3.5

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Mol	Chain	Res	Type	RSRZ
1	I	44	GLU	3.5
1	Y	12	ALA	3.5
2	X	413	ASP	3.5
1	W	228	SER	3.5
1	I	48	ARG	3.5
1	K	131	GLY	3.5
1	S	44	GLU	3.4
1	A	172	ALA	3.4
1	B	205	VAL	3.4
2	N	412	SER	3.4
2	P	399	LEU	3.4
1	1	206	ALA	3.4
1	Q	173	GLU	3.4
1	K	135	ARG	3.4
2	X	391	LEU	3.4
2	T	391	LEU	3.3
1	O	13	MET	3.3
1	K	133	THR	3.3
1	A	206	ALA	3.3
1	I	10	GLU	3.3
1	B	133	THR	3.3
1	Y	15	GLU	3.3
1	M	11	GLN	3.3
1	1	228	SER	3.3
1	B	171	TYR	3.3
1	D	133	THR	3.3
1	Y	48	ARG	3.2
1	D	227	GLY	3.2
1	Q	11	GLN	3.2
1	U	11	GLN	3.2
1	1	9	PRO	3.2
1	W	135	ARG	3.2
1	U	131	GLY	3.2
1	W	26	ARG	3.2
1	A	177	LEU	3.2
1	A	186	ALA	3.2
2	2	391	LEU	3.1
1	D	179	ASP	3.1
1	U	228	SER	3.1
1	W	169	GLU	3.1
1	1	205	VAL	3.1
1	F	203	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
1	I	231	GLN	3.1
1	1	48	ARG	3.1
2	L	400	ALA	3.1
1	A	165	ASN	3.1
1	U	8	SER	3.1
1	1	11	GLN	3.1
1	Q	131	GLY	3.1
1	D	172	ALA	3.1
1	Y	231	GLN	3.1
1	M	179	ASP	3.0
1	M	10	GLU	3.0
1	M	165	ASN	3.0
1	1	169	GLU	3.0
1	I	206	ALA	3.0
1	I	15	GLU	3.0
1	M	131	GLY	3.0
1	O	135	ARG	3.0
1	O	231	GLN	3.0
1	A	131	GLY	2.9
1	D	27	ALA	2.9
1	Y	186	ALA	2.9
1	Q	179	ASP	2.9
1	B	169	GLU	2.9
1	S	135	ARG	2.9
1	K	173	GLU	2.9
1	Q	36	ALA	2.9
1	Y	165	ASN	2.9
1	K	48	ARG	2.9
2	X	412	SER	2.9
1	W	231	GLN	2.9
1	Y	206	ALA	2.9
2	2	392	ALA	2.9
1	A	227	GLY	2.9
2	C	412	SER	2.8
2	G	392	ALA	2.8
1	F	162	PRO	2.8
1	F	169	GLU	2.8
1	I	161	GLU	2.8
2	H	412	SER	2.8
1	I	133	THR	2.8
2	J	413	ASP	2.8
1	W	229	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
1	W	165	ASN	2.8
1	S	171	TYR	2.8
1	A	189	ARG	2.8
1	D	158	GLY	2.8
1	K	231	GLN	2.8
2	2	412	SER	2.8
1	Q	203	LEU	2.8
1	W	181	LEU	2.8
1	D	10	GLU	2.8
1	W	12	ALA	2.8
1	W	11	GLN	2.8
1	S	15	GLU	2.8
1	K	205	VAL	2.8
1	O	133	THR	2.8
2	2	486	LEU	2.7
1	K	229	ALA	2.7
2	Z	432	GLU	2.7
2	L	391	LEU	2.7
1	K	226	THR	2.7
1	U	232	ALA	2.7
1	D	37	GLY	2.7
1	Y	174	ASN	2.7
1	M	13	MET	2.7
1	S	160	THR	2.7
1	Y	172	ALA	2.7
1	Y	180	ALA	2.7
1	A	161	GLU	2.7
1	K	161	GLU	2.7
1	U	44	GLU	2.7
1	D	231	GLN	2.7
1	M	46	PRO	2.7
1	M	161	GLU	2.7
1	W	188	LEU	2.7
1	I	160	THR	2.7
1	K	26	ARG	2.7
1	M	182	ARG	2.7
2	V	400	ALA	2.7
2	V	391	LEU	2.7
1	B	10	GLU	2.7
1	W	182	ARG	2.7
1	K	153	PHE	2.7
1	W	184	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
1	I	189	ARG	2.6
1	D	165	ASN	2.6
1	1	165	ASN	2.6
1	K	14	ARG	2.6
2	J	433	GLU	2.6
1	A	188	LEU	2.6
2	P	391	LEU	2.6
1	S	13	MET	2.6
1	W	173	GLU	2.6
1	1	232	ALA	2.6
2	X	400	ALA	2.6
1	I	14	ARG	2.6
1	A	231	GLN	2.6
1	1	133	THR	2.6
1	D	228	SER	2.6
1	K	186	ALA	2.6
2	T	392	ALA	2.6
1	1	231	GLN	2.6
1	Q	14	ARG	2.6
2	L	399	LEU	2.6
1	1	152	HIS	2.6
1	D	205	VAL	2.5
2	N	330	ASP	2.5
1	W	203	LEU	2.5
1	D	178	THR	2.5
1	M	231	GLN	2.5
1	D	18	GLU	2.5
1	Y	182	ARG	2.5
1	K	184	ALA	2.5
1	S	206	ALA	2.5
2	T	400	ALA	2.5
1	U	169	GLU	2.5
1	O	11	GLN	2.5
1	B	14	ARG	2.5
1	B	135	ARG	2.5
1	Q	182	ARG	2.5
1	F	179	ASP	2.5
1	K	172	ALA	2.5
1	1	172	ALA	2.5
1	Y	111	PHE	2.5
1	F	173	GLU	2.5
1	S	113	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
1	W	44	GLU	2.5
1	S	133	THR	2.5
2	2	425	ALA	2.5
1	S	161	GLU	2.5
1	D	168	LYS	2.5
1	1	159	THR	2.5
1	D	171	TYR	2.5
1	A	13	MET	2.5
1	Q	37	GLY	2.5
2	Z	412	SER	2.5
1	A	133	THR	2.5
1	B	11	GLN	2.5
1	O	165	ASN	2.5
1	S	165	ASN	2.5
1	S	146	SER	2.5
1	O	10	GLU	2.4
1	U	26	ARG	2.4
1	I	13	MET	2.4
2	T	412	SER	2.4
1	Q	181	LEU	2.4
1	Y	128	ALA	2.4
1	Q	113	GLU	2.4
1	A	205	VAL	2.4
1	Q	165	ASN	2.4
2	J	399	LEU	2.4
1	K	150	GLU	2.4
2	C	519	GLU	2.4
1	K	189	ARG	2.4
1	S	12	ALA	2.4
1	Y	189	ARG	2.4
2	P	425	ALA	2.4
1	A	203	LEU	2.4
1	S	10	GLU	2.4
1	W	48	ARG	2.4
1	Y	149	ASP	2.4
1	1	14	ARG	2.4
1	K	152	HIS	2.4
1	B	182	ARG	2.4
1	A	141	ILE	2.4
1	M	44	GLU	2.4
1	U	15	GLU	2.4
1	D	125	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
2	R	400	ALA	2.4
1	D	26	ARG	2.3
1	I	182	ARG	2.3
1	F	161	GLU	2.3
1	W	159	THR	2.3
1	M	28	LYS	2.3
1	M	48	ARG	2.3
2	C	432	GLU	2.3
1	D	207	SER	2.3
1	U	148	ALA	2.3
1	W	225	ILE	2.3
1	O	169	GLU	2.3
1	U	161	GLU	2.3
2	X	330	ASP	2.3
2	Z	519	GLU	2.3
2	2	330	ASP	2.3
1	A	171	TYR	2.3
1	F	8	SER	2.3
1	W	178	THR	2.3
1	A	230	LEU	2.3
1	Q	233	LEU	2.3
2	C	391	LEU	2.3
2	N	519	GLU	2.3
1	Q	135	ARG	2.3
1	K	167	LEU	2.3
2	G	330	ASP	2.3
2	Z	414	PRO	2.3
2	2	400	ALA	2.3
2	L	433	GLU	2.3
1	M	171	TYR	2.3
1	M	162	PRO	2.3
1	K	12	ALA	2.2
2	P	392	ALA	2.2
1	Q	44	GLU	2.2
1	U	234	LEU	2.2
1	Y	161	GLU	2.2
2	C	400	ALA	2.2
1	Y	150	GLU	2.2
1	M	14	ARG	2.2
1	O	48	ARG	2.2
1	O	189	ARG	2.2
1	S	153	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
1	F	171	TYR	2.2
1	W	10	GLU	2.2
1	A	14	ARG	2.2
1	I	131	GLY	2.2
1	Y	167	LEU	2.2
1	K	113	GLU	2.2
1	O	154	VAL	2.2
1	B	179	ASP	2.2
1	O	148	ALA	2.2
1	O	182	ARG	2.2
1	1	135	ARG	2.2
1	I	234	LEU	2.2
1	U	18	GLU	2.2
1	1	203	LEU	2.2
1	O	179	ASP	2.2
1	K	206	ALA	2.2
1	K	111	PHE	2.2
1	Q	50	LEU	2.2
1	O	160	THR	2.2
1	F	206	ALA	2.1
1	W	13	MET	2.1
1	1	161	GLU	2.1
1	B	152	HIS	2.1
1	B	161	GLU	2.1
1	F	113	GLU	2.1
1	Y	137	GLU	2.1
2	E	392	ALA	2.1
2	J	400	ALA	2.1
1	Q	48	ARG	2.1
1	Y	135	ARG	2.1
1	Y	234	LEU	2.1
1	O	173	GLU	2.1
1	I	135	ARG	2.1
1	1	44	GLU	2.1
1	U	153	PHE	2.1
1	M	228	SER	2.1
1	S	14	ARG	2.1
1	K	180	ALA	2.1
1	M	175	ALA	2.1
1	W	232	ALA	2.1
2	P	330	ASP	2.1
1	I	181	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	S	227	GLY	2.1
1	F	15	GLU	2.1
1	M	232	ALA	2.1
1	K	177	LEU	2.1
1	S	131	GLY	2.1
1	Q	228	SER	2.1
2	J	330	ASP	2.1
1	F	232	ALA	2.1
2	H	425	ALA	2.1
1	S	11	GLN	2.1
1	I	165	ASN	2.1
1	K	44	GLU	2.1
1	S	204	GLY	2.1
1	A	179	ASP	2.1
1	S	179	ASP	2.1
2	J	392	ALA	2.0
1	I	113	GLU	2.0
1	K	18	GLU	2.0
1	K	42	VAL	2.0
1	W	113	GLU	2.0
1	D	130	TYR	2.0
1	I	11	GLN	2.0
1	I	173	GLU	2.0
2	L	392	ALA	2.0
1	K	185	VAL	2.0
1	K	130	TYR	2.0
1	K	171	TYR	2.0
1	O	228	SER	2.0
1	A	10	GLU	2.0
2	2	519	GLU	2.0
1	M	185	VAL	2.0
1	B	15	GLU	2.0
1	1	163	ILE	2.0
1	F	182	ARG	2.0
1	K	97	ARG	2.0
1	Y	153	PHE	2.0
1	Y	160	THR	2.0
1	Q	216	ASN	2.0

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	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 (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
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
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
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

There are no such residues in this entry.