



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 08:12 am GMT

PDB ID : 3MI0  
Title : Crystal Structure of Mycobacterium Tuberculosis Proteasome at 2.2 Å  
Authors : Li, D.; Li, H.  
Deposited on : 2010-04-09  
Resolution : 2.20 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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : recalc28949

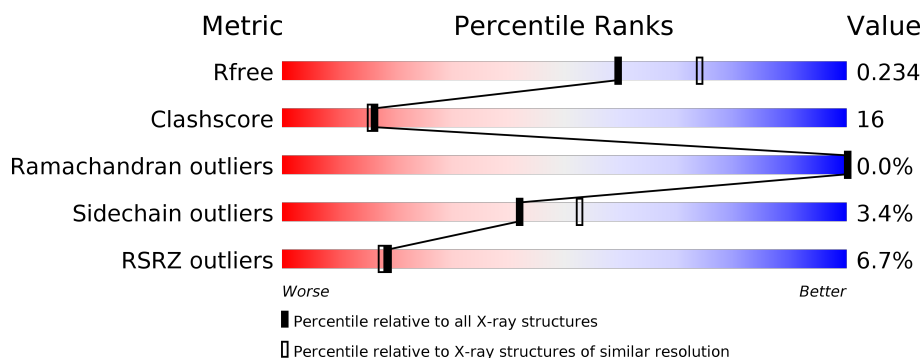
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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))
$R_{free}$	100719	4002 (2.20-2.20)
Clashscore	112137	4730 (2.20-2.20)
Ramachandran outliers	110173	4656 (2.20-2.20)
Sidechain outliers	110143	4657 (2.20-2.20)
RSRZ outliers	101464	4033 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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>7%</div> <div>64%</div> <div>21%</div> <div>13%</div> </div>
1	A	248	<div> <div>12%</div> <div>60%</div> <div>24%</div> <div>13%</div> </div>
1	B	248	<div> <div>6%</div> <div>59%</div> <div>24%</div> <div>14%</div> </div>
1	D	248	<div> <div>24%</div> <div>50%</div> <div>34%</div> <div>14%</div> </div>
1	F	248	<div> <div>7%</div> <div>60%</div> <div>27%</div> <div>11%</div> </div>
1	I	248	<div> <div>11%</div> <div>54%</div> <div>31%</div> <div>13%</div> </div>

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	DMF	1	249	-	-	-	X
3	DMF	2	101	-	-	-	X
3	DMF	2	108	-	-	X	X
3	DMF	2	112	-	-	X	X
3	DMF	2	4	-	-	X	X
3	DMF	2	49	-	-	-	X
3	DMF	2	52	-	-	-	X
3	DMF	2	57	-	-	-	X
3	DMF	2	87	-	-	-	X
3	DMF	A	249	-	-	-	X
3	DMF	A	250	-	-	-	X
3	DMF	B	249	-	-	-	X
3	DMF	B	250	-	-	-	X
3	DMF	C	103	-	-	X	X
3	DMF	C	47	-	-	-	X
3	DMF	C	63	-	-	-	X
3	DMF	C	88	-	-	-	X
3	DMF	D	249	-	-	-	X
3	DMF	D	250	-	-	-	X
3	DMF	D	251	-	-	X	X
3	DMF	D	252	-	-	-	X
3	DMF	D	253	-	-	-	X
3	DMF	E	20	-	-	X	X
3	DMF	E	28	-	-	-	X
3	DMF	E	53	-	-	-	X
3	DMF	E	75	-	-	X	X
3	DMF	F	249	-	-	-	X
3	DMF	F	250	-	-	-	X
3	DMF	F	251	-	-	-	X
3	DMF	G	111	-	-	-	X
3	DMF	G	119	-	-	X	X
3	DMF	G	12	-	-	X	X
3	DMF	G	24	-	-	-	X
3	DMF	G	62	-	-	-	X
3	DMF	G	64	-	-	X	X
3	DMF	G	70	-	-	-	X
3	DMF	G	77	-	-	-	X
3	DMF	G	98	-	-	-	X
3	DMF	H	117	-	-	-	X
3	DMF	H	43	-	-	X	X
3	DMF	H	72	-	-	-	X
3	DMF	I	249	-	-	-	X
3	DMF	I	250	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	DMF	J	110	-	-	-	X
3	DMF	J	123	-	-	X	X
3	DMF	J	45	-	-	-	X
3	DMF	K	249	-	-	-	X
3	DMF	K	250	-	-	X	X
3	DMF	K	251	-	-	-	X
3	DMF	L	36	-	-	-	X
3	DMF	L	81	-	-	-	X
3	DMF	L	97	-	-	X	X
3	DMF	M	249	-	-	-	X
3	DMF	M	250	-	-	-	X
3	DMF	M	251	-	-	-	X
3	DMF	M	252	-	-	-	X
3	DMF	N	104	-	-	X	X
3	DMF	N	118	-	-	X	X
3	DMF	N	22	-	-	X	-
3	DMF	N	90	-	-	X	X
3	DMF	N	93	-	-	X	X
3	DMF	O	249	-	-	-	X
3	DMF	O	250	-	-	-	X
3	DMF	O	251	-	-	-	X
3	DMF	P	107	-	-	X	X
3	DMF	P	14	-	-	X	X
3	DMF	P	2	-	-	-	X
3	DMF	P	56	-	-	-	X
3	DMF	P	60	-	-	-	X
3	DMF	Q	249	-	-	-	X
3	DMF	Q	250	-	-	X	X
3	DMF	Q	251	-	-	-	X
3	DMF	R	59	-	-	X	X
3	DMF	R	89	-	-	-	X
3	DMF	R	95	-	-	-	X
3	DMF	S	249	-	-	-	X
3	DMF	S	250	-	-	-	X
3	DMF	T	10	-	-	-	X
3	DMF	T	102	-	-	-	X
3	DMF	T	113	-	-	X	X
3	DMF	T	115	-	-	-	X
3	DMF	T	29	-	-	-	X
3	DMF	T	84	-	-	-	X
3	DMF	U	249	-	-	-	X
3	DMF	U	250	-	-	X	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	DMF	V	109	-	-	-	X
3	DMF	V	116	-	-	X	-
3	DMF	V	120	-	-	X	X
3	DMF	V	27	-	-	X	X
3	DMF	V	32	-	-	X	X
3	DMF	V	39	-	-	-	X
3	DMF	V	42	-	-	X	X
3	DMF	V	82	-	-	-	X
3	DMF	V	83	-	-	X	X
3	DMF	W	249	-	-	-	X
3	DMF	W	250	-	-	X	X
3	DMF	X	122	-	-	-	X
3	DMF	X	15	-	-	-	X
3	DMF	X	16	-	-	-	X
3	DMF	X	41	-	-	-	X
3	DMF	Y	249	-	-	-	X
3	DMF	Y	250	-	-	-	X
3	DMF	Y	251	-	-	-	X
3	DMF	Z	114	-	-	-	X
3	DMF	Z	18	-	-	-	X
3	DMF	Z	54	-	-	-	X
3	DMF	Z	94	-	-	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 50080 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 subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	215	Total	C	N	O	S	0	0	0
			1654	1035	303	313	3			
1	B	213	Total	C	N	O	S	0	0	0
			1643	1028	301	311	3			
1	D	214	Total	C	N	O	S	0	0	0
			1650	1033	302	312	3			
1	F	220	Total	C	N	O	S	0	0	0
			1699	1068	308	320	3			
1	I	216	Total	C	N	O	S	0	0	0
			1669	1048	304	314	3			
1	K	216	Total	C	N	O	S	0	0	0
			1666	1045	304	314	3			
1	M	216	Total	C	N	O	S	0	0	0
			1666	1045	304	314	3			
1	O	216	Total	C	N	O	S	0	0	0
			1666	1045	304	314	3			
1	Q	215	Total	C	N	O	S	0	0	0
			1658	1039	303	313	3			
1	S	216	Total	C	N	O	S	0	0	0
			1665	1044	304	314	3			
1	U	216	Total	C	N	O	S	0	0	0
			1662	1041	304	314	3			
1	W	216	Total	C	N	O	S	0	0	0
			1669	1048	304	314	3			
1	Y	216	Total	C	N	O	S	0	0	0
			1666	1045	304	314	3			
1	1	215	Total	C	N	O	S	0	0	0
			1658	1039	303	313	3			

- Molecule 2 is a protein called Proteasome subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	222	Total	C	N	O	S	0	0	0
			1638	1027	282	324	5			
2	E	223	Total	C	N	O	S	0	0	0
			1642	1029	283	325	5			
2	G	222	Total	C	N	O	S	0	0	0
			1638	1027	282	324	5			
2	H	222	Total	C	N	O	S	0	0	0
			1638	1027	282	324	5			
2	J	222	Total	C	N	O	S	0	0	0
			1638	1027	282	324	5			
2	L	223	Total	C	N	O	S	0	0	0
			1642	1029	283	325	5			
2	N	222	Total	C	N	O	S	0	0	0
			1638	1027	282	324	5			
2	P	222	Total	C	N	O	S	0	0	0
			1638	1027	282	324	5			
2	R	239	Total	C	N	O	S	0	0	0
			1767	1103	310	349	5			
2	T	223	Total	C	N	O	S	0	0	0
			1642	1029	283	325	5			
2	V	239	Total	C	N	O	S	0	0	0
			1767	1103	310	349	5			
2	X	223	Total	C	N	O	S	0	0	0
			1642	1029	283	325	5			
2	Z	223	Total	C	N	O	S	0	0	0
			1642	1029	283	325	5			
2	2	223	Total	C	N	O	S	0	0	0
			1642	1029	283	325	5			

There are 84 discrepancies between the modelled and reference sequences:

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

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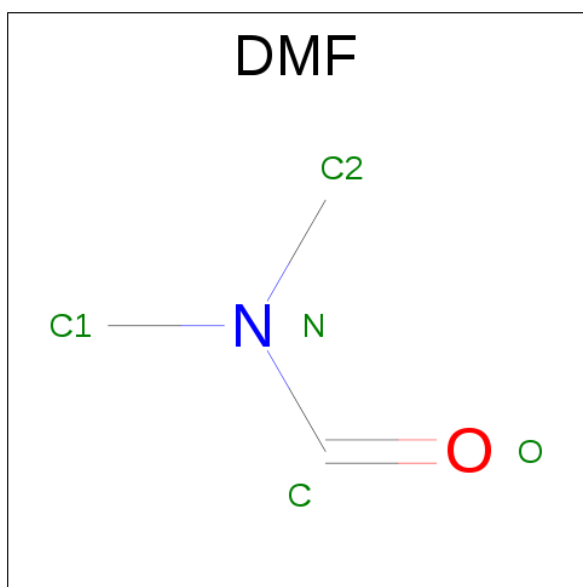
Chain	Residue	Modelled	Actual	Comment	Reference
G	535	HIS	-	EXPRESSION TAG	UNP O33245
G	536	HIS	-	EXPRESSION TAG	UNP O33245
G	537	HIS	-	EXPRESSION TAG	UNP O33245
G	538	HIS	-	EXPRESSION TAG	UNP O33245
G	539	HIS	-	EXPRESSION TAG	UNP O33245
G	540	HIS	-	EXPRESSION TAG	UNP O33245
H	535	HIS	-	EXPRESSION TAG	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	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	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	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	535	HIS	-	EXPRESSION TAG	UNP O33245
P	536	HIS	-	EXPRESSION TAG	UNP O33245
P	537	HIS	-	EXPRESSION TAG	UNP O33245
P	538	HIS	-	EXPRESSION TAG	UNP O33245
P	539	HIS	-	EXPRESSION TAG	UNP O33245
P	540	HIS	-	EXPRESSION TAG	UNP O33245
R	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

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

- Molecule 3 is DIMETHYLFORMAMIDE (three-letter code: DMF) (formula: C<sub>3</sub>H<sub>7</sub>NO).



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

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	D	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		
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		
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	F	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	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		

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

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
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	O	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	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	Q	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		

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

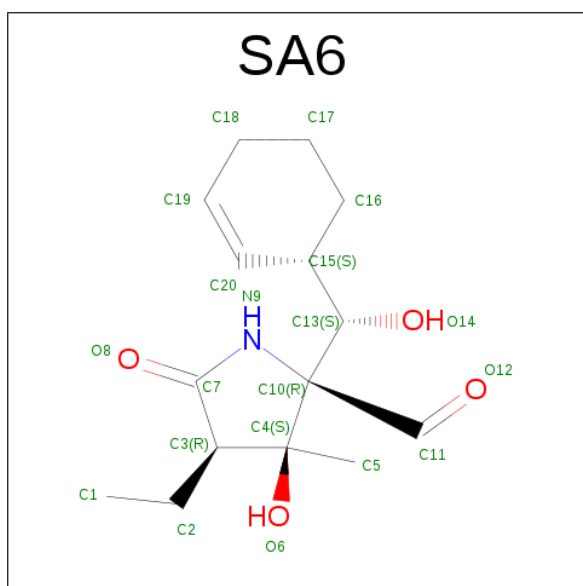
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	2	1	Total	C	N	O	0	0
			5	3	1	1		
3	2	1	Total	C	N	O	0	0
			5	3	1	1		
3	2	1	Total	C	N	O	0	0
			5	3	1	1		
3	2	1	Total	C	N	O	0	0
			5	3	1	1		

- Molecule 4 is (2R,3S,4R)-2-[(S)-(1S)-CYCLOHEX-2-EN-1-YL(HYDROXY)METHYL]-4-ETHYL-3-HYDROXY-3-METHYL-5-OPYRROLIDINE-2-CARBALDEHYDE (three-letter code: SA6) (formula: C<sub>15</sub>H<sub>23</sub>NO<sub>4</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	C	1	Total	C	N	O	0	0
			20	15	1	4		
4	E	1	Total	C	N	O	0	0
			20	15	1	4		
4	G	1	Total	C	N	O	0	0
			20	15	1	4		
4	H	1	Total	C	N	O	0	0
			20	15	1	4		
4	J	1	Total	C	N	O	0	0
			20	15	1	4		
4	L	1	Total	C	N	O	0	0
			20	15	1	4		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	N	1	Total	C	N	O	0	0
			20	15	1	4		
4	P	1	Total	C	N	O	0	0
			20	15	1	4		
4	R	1	Total	C	N	O	0	0
			20	15	1	4		
4	T	1	Total	C	N	O	0	0
			20	15	1	4		
4	V	1	Total	C	N	O	0	0
			20	15	1	4		
4	X	1	Total	C	N	O	0	0
			20	15	1	4		
4	Z	1	Total	C	N	O	0	0
			20	15	1	4		
4	2	1	Total	C	N	O	0	0
			20	15	1	4		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	43	Total	O	0	0
			43	43		
5	B	41	Total	O	0	0
			41	41		
5	C	163	Total	O	0	0
			163	163		
5	D	40	Total	O	0	0
			40	40		
5	E	166	Total	O	0	0
			166	166		
5	F	58	Total	O	0	0
			58	58		
5	G	131	Total	O	0	0
			131	131		
5	H	148	Total	O	0	0
			148	148		
5	I	52	Total	O	0	0
			52	52		
5	J	142	Total	O	0	0
			142	142		
5	K	45	Total	O	0	0
			45	45		

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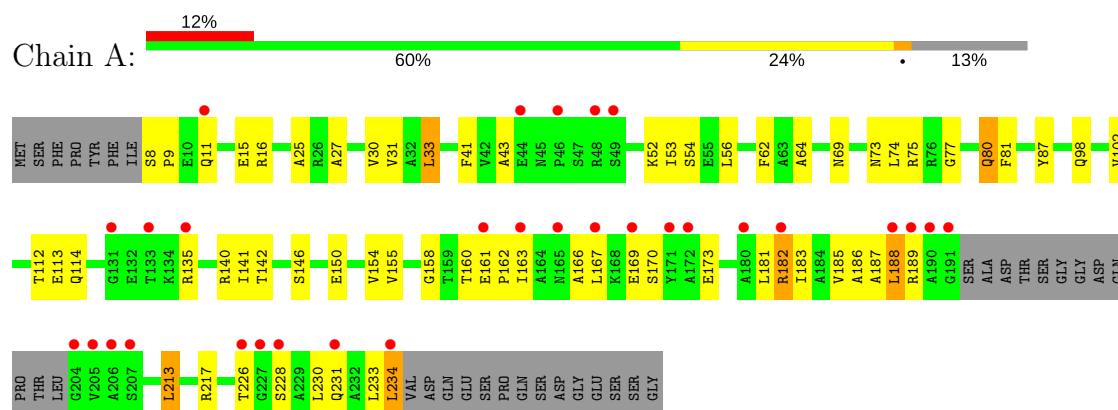
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	L	153	Total 153	O 153	0	0
5	M	40	Total 40	O 40	0	0
5	N	154	Total 154	O 154	0	0
5	O	47	Total 47	O 47	0	0
5	P	139	Total 139	O 139	0	0
5	Q	38	Total 38	O 38	0	0
5	R	170	Total 170	O 170	0	0
5	S	42	Total 42	O 42	0	0
5	T	116	Total 116	O 116	0	0
5	U	49	Total 49	O 49	0	0
5	V	177	Total 177	O 177	0	0
5	W	35	Total 35	O 35	0	0
5	X	150	Total 150	O 150	0	0
5	Y	28	Total 28	O 28	0	0
5	Z	123	Total 123	O 123	0	0
5	1	47	Total 47	O 47	0	0
5	2	143	Total 143	O 143	0	0

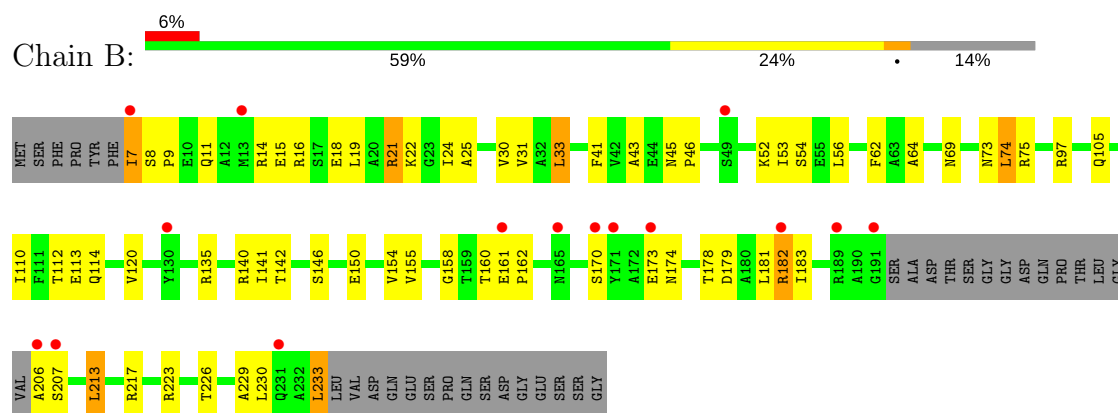
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

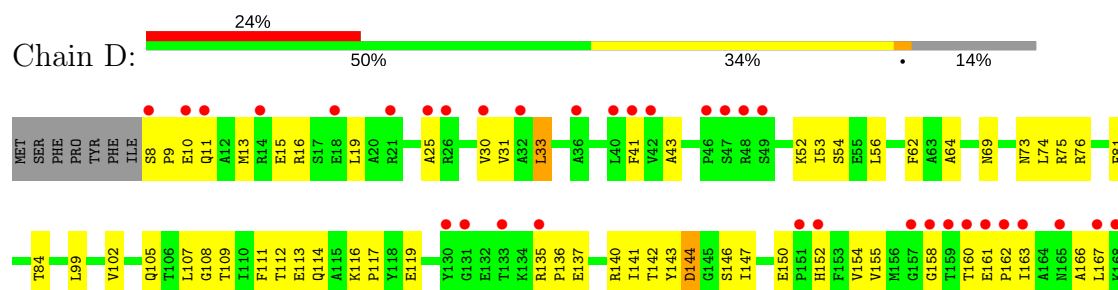
#### • Molecule 1: Proteasome subunit alpha



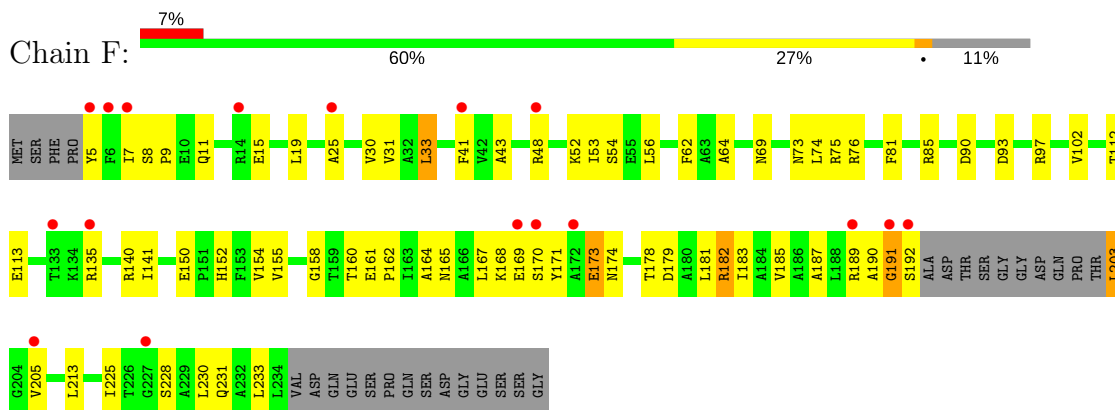
#### • Molecule 1: Proteasome subunit alpha



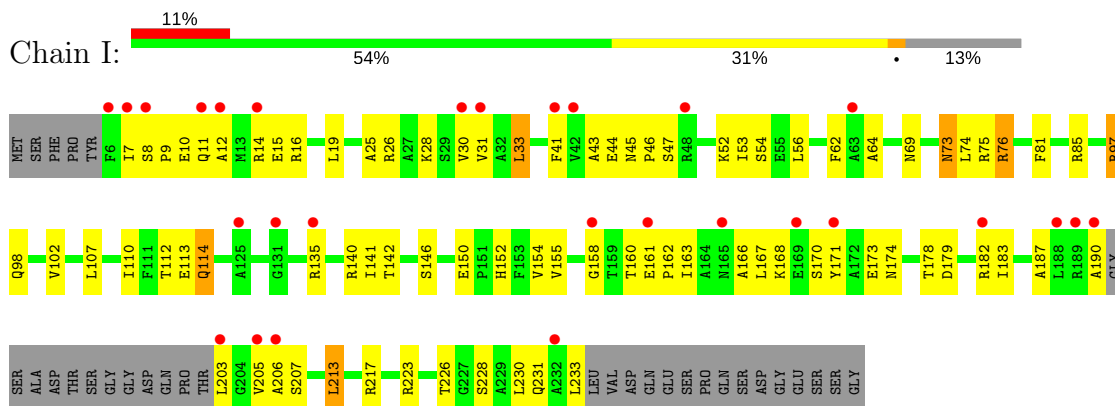
#### • Molecule 1: Proteasome subunit alpha



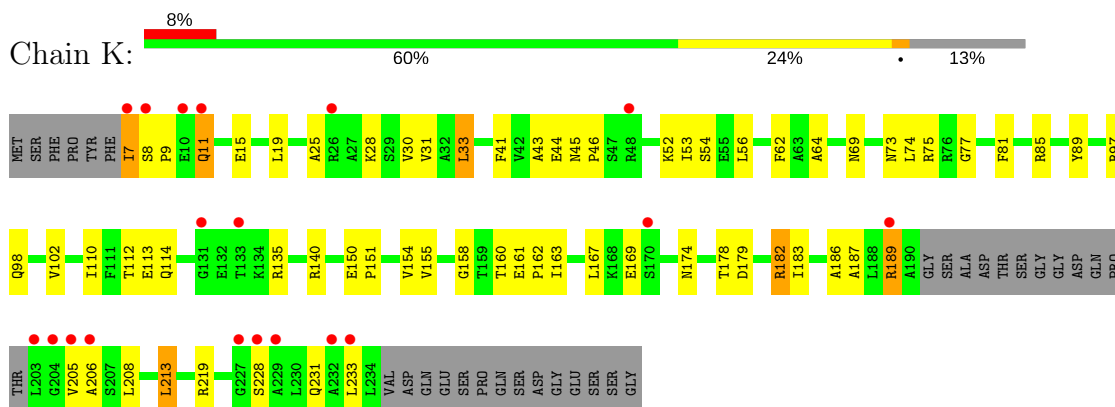
- Molecule 1: Proteasome subunit alpha



- Molecule 1: Proteasome subunit alpha

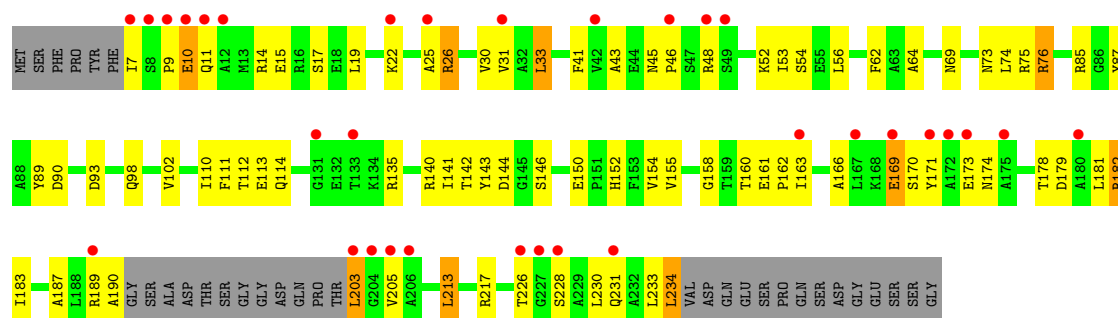


- Molecule 1: Proteasome subunit alpha

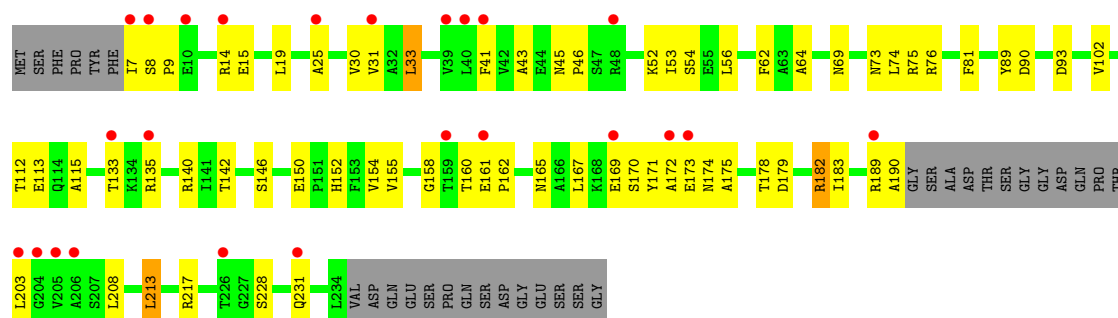


- Molecule 1: Proteasome subunit alpha

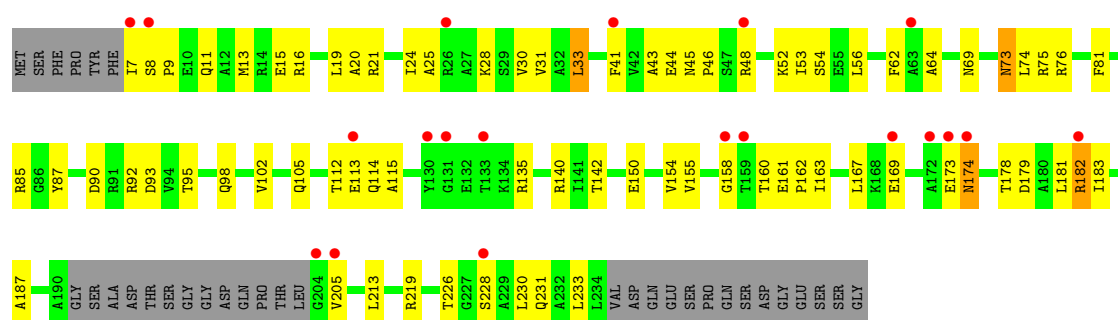




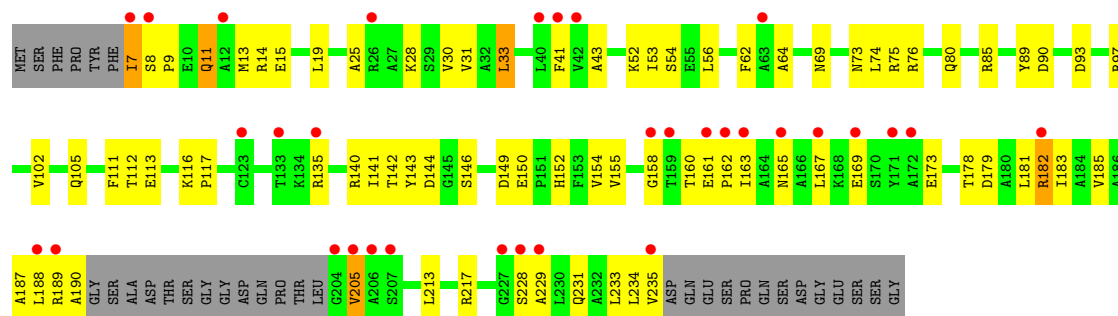
• Molecule 1: Proteasome subunit alpha



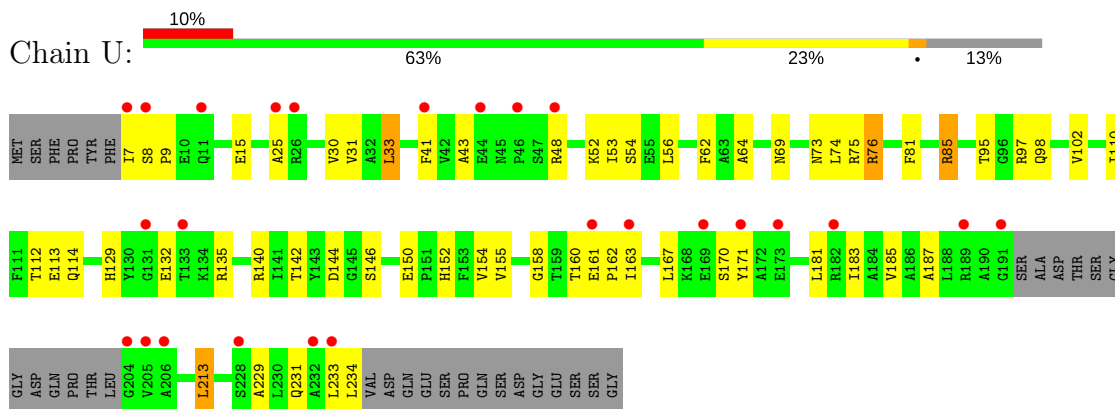
• Molecule 1: Proteasome subunit alpha



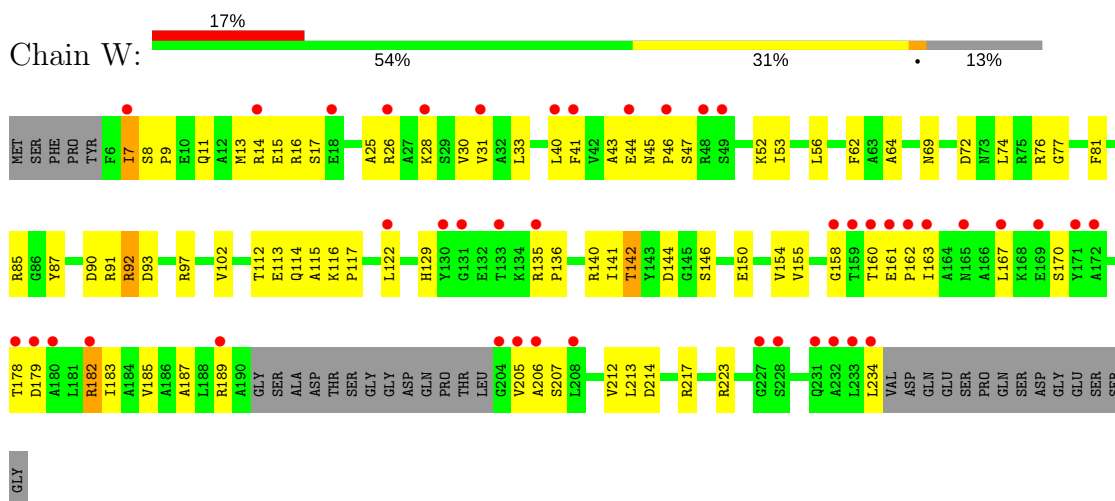
• Molecule 1: Proteasome subunit alpha



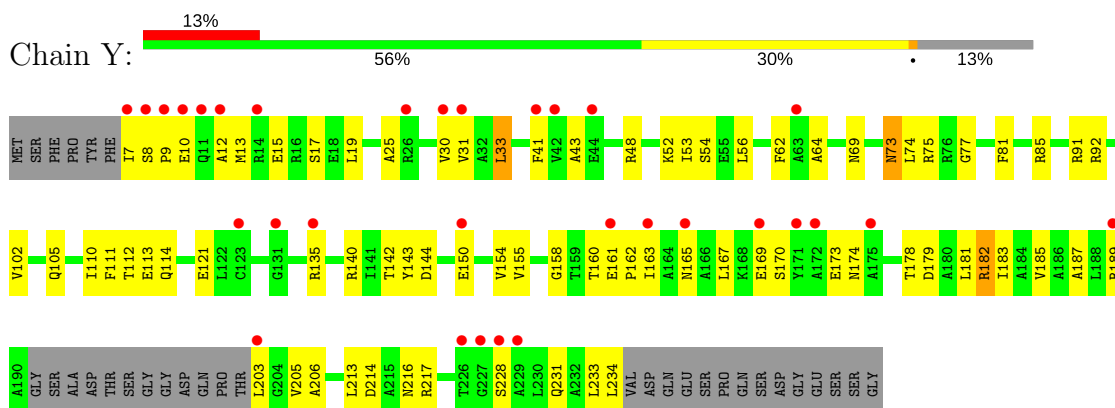
- Molecule 1: Proteasome subunit alpha



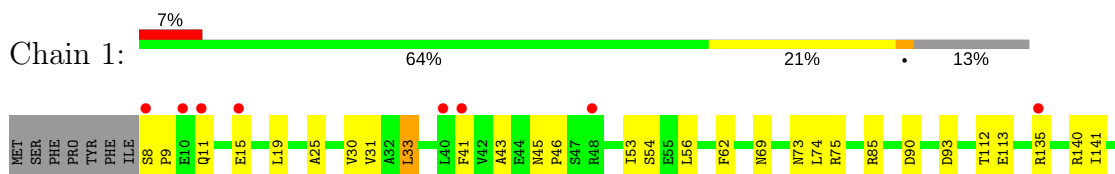
- Molecule 1: Proteasome subunit alpha

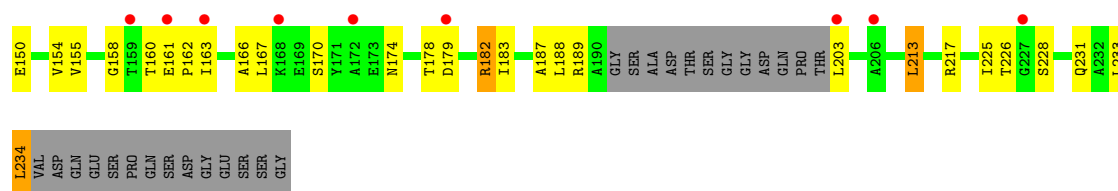


- Molecule 1: Proteasome subunit alpha

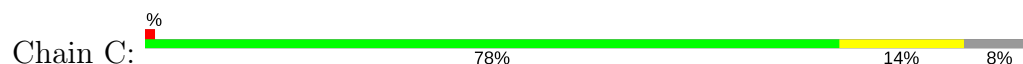


- Molecule 1: Proteasome subunit alpha

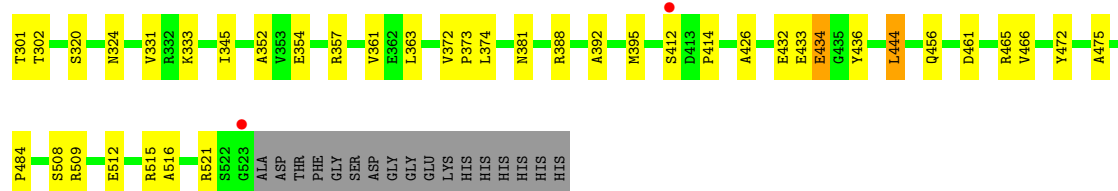
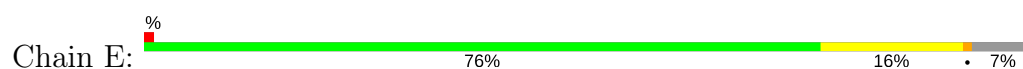




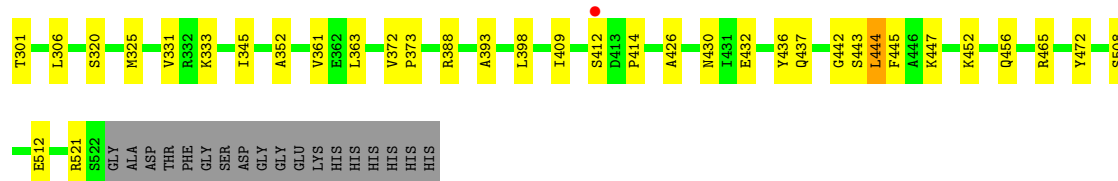
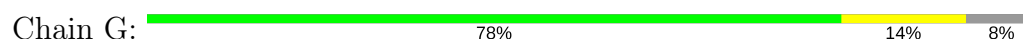
• Molecule 2: Proteasome subunit beta



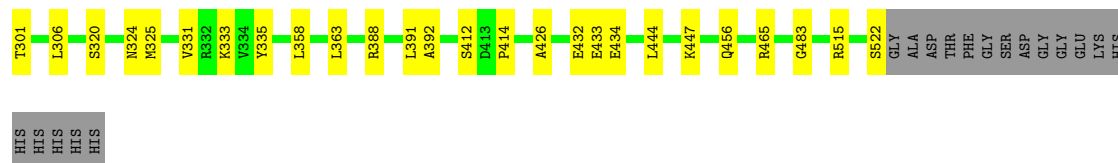
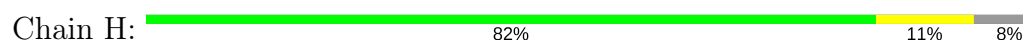
• Molecule 2: Proteasome subunit beta



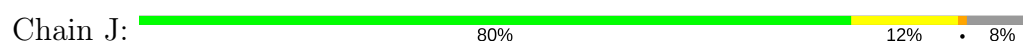
• Molecule 2: Proteasome subunit beta



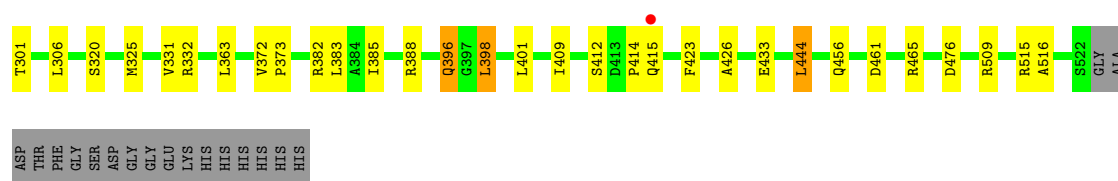
• Molecule 2: Proteasome subunit beta



• Molecule 2: Proteasome subunit beta

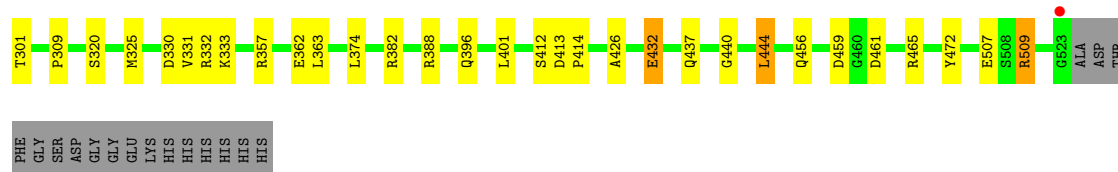






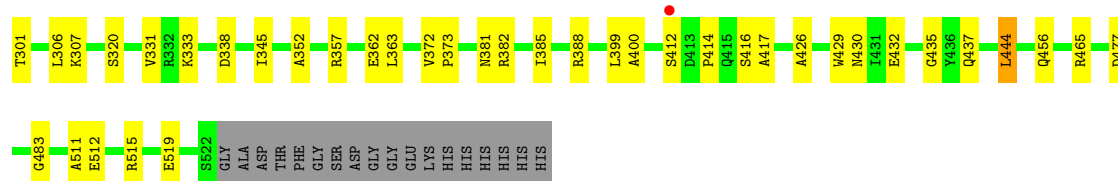
• Molecule 2: Proteasome subunit beta

Chain L: 80% 12% 7%



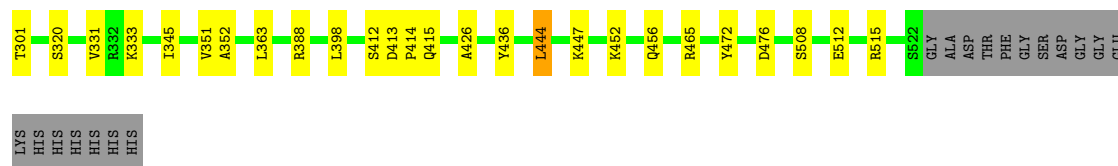
• Molecule 2: Proteasome subunit beta

Chain N: 76% 16% 8%



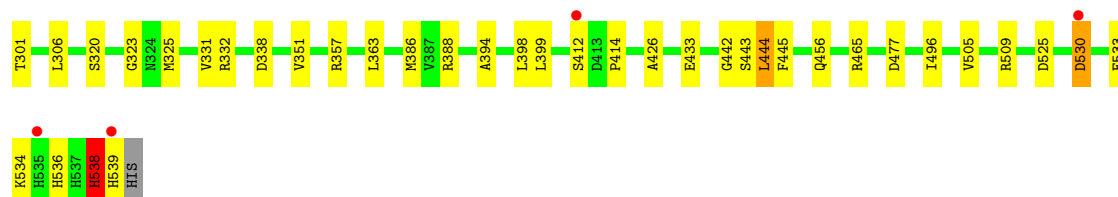
• Molecule 2: Proteasome subunit beta

Chain P: 82% 10% 8%



• Molecule 2: Proteasome subunit beta

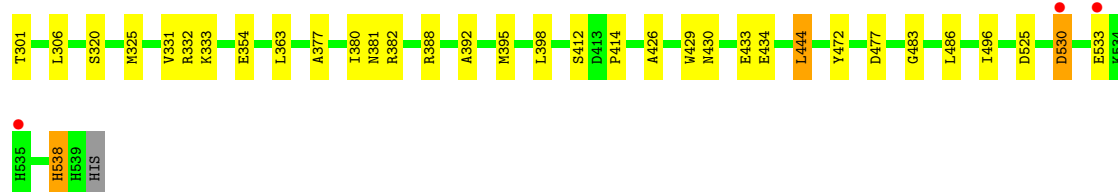
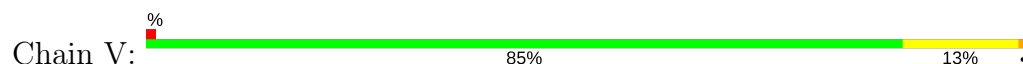
Chain R: 84% 14% 2%



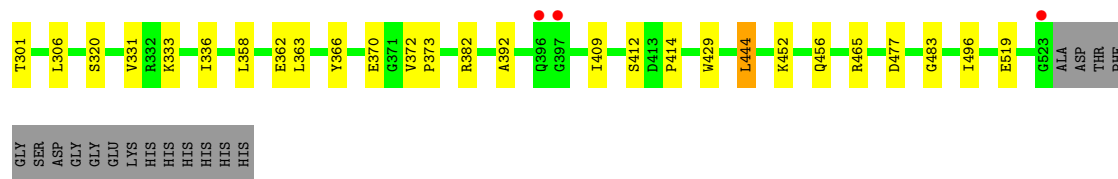
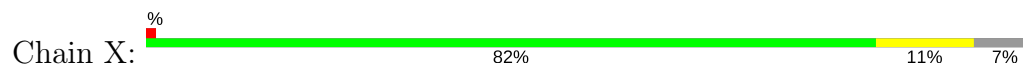
• Molecule 2: Proteasome subunit beta

Chain T: 81% 12% 7%

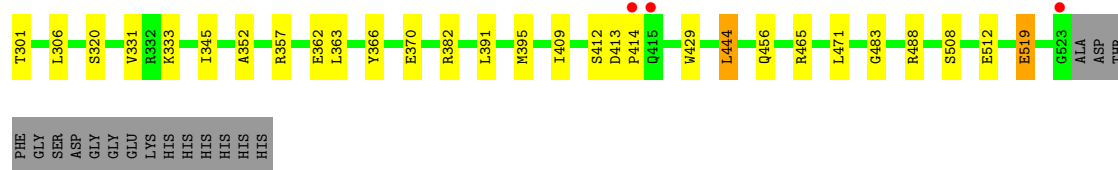
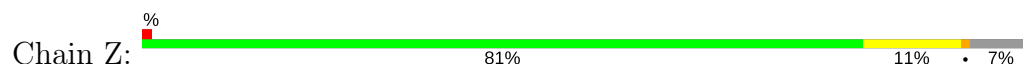
- Molecule 2: Proteasome subunit beta



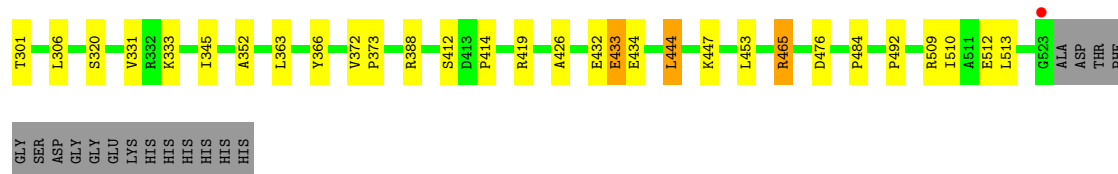
- Molecule 2: Proteasome subunit beta



- Molecule 2: Proteasome subunit beta



- Molecule 2: Proteasome subunit beta



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	170.37Å 118.44Å 195.25Å 90.00° 113.02° 90.00°	Depositor
Resolution (Å)	24.95 – 2.20 25.11 – 2.12	Depositor EDS
% Data completeness (in resolution range)	92.0 (24.95-2.20) 89.2 (25.11-2.12)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.78 (at 2.11Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, $R_{free}$	0.205 , 0.234 0.205 , 0.234	Depositor DCC
$R_{free}$ test set	16561 reflections (4.98%)	DCC
Wilson B-factor (Å <sup>2</sup> )	22.6	Xtriage
Anisotropy	0.230	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 56.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.008 for h,-k,-h-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	50080	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.53% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SA6, 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	0.53	0/1683	0.73	1/2274 (0.0%)
1	A	0.49	0/1679	0.72	1/2268 (0.0%)
1	B	0.52	0/1668	0.71	1/2253 (0.0%)
1	D	0.46	0/1675	0.69	1/2263 (0.0%)
1	F	0.51	0/1726	0.74	2/2332 (0.1%)
1	I	0.51	0/1695	0.73	4/2290 (0.2%)
1	K	0.51	0/1691	0.71	1/2285 (0.0%)
1	M	0.51	0/1691	0.74	2/2285 (0.1%)
1	O	0.51	0/1691	0.72	1/2285 (0.0%)
1	Q	0.47	0/1683	0.69	1/2274 (0.0%)
1	S	0.50	0/1690	0.72	2/2284 (0.1%)
1	U	0.49	0/1687	0.71	3/2279 (0.1%)
1	W	0.44	0/1695	0.68	1/2290 (0.0%)
1	Y	0.48	0/1691	0.72	1/2285 (0.0%)
2	2	0.65	0/1666	0.79	0/2259
2	C	0.71	0/1662	0.84	2/2254 (0.1%)
2	E	0.73	0/1666	0.81	0/2259
2	G	0.66	0/1662	0.77	0/2254
2	H	0.70	0/1662	0.79	0/2254
2	J	0.71	0/1662	0.81	0/2254
2	L	0.70	0/1666	0.80	0/2259
2	N	0.69	0/1662	0.81	1/2254 (0.0%)
2	P	0.69	0/1662	0.79	0/2254
2	R	0.71	0/1797	0.81	3/2435 (0.1%)
2	T	0.66	0/1666	0.77	1/2259 (0.0%)
2	V	0.70	0/1797	0.78	1/2435 (0.0%)
2	X	0.64	0/1666	0.78	0/2259
2	Z	0.62	0/1666	0.75	0/2259
All	All	0.60	0/47207	0.76	30/63895 (0.0%)

There are no bond length outliers.

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Y	213	LEU	N-CA-C	-5.99	94.82	111.00
2	R	338	ASP	CB-CG-OD1	5.80	123.52	118.30
1	M	76	ARG	NE-CZ-NH2	-5.77	117.42	120.30
1	I	213	LEU	N-CA-C	-5.71	95.60	111.00
1	K	213	LEU	N-CA-C	-5.70	95.61	111.00
2	C	338	ASP	CB-CG-OD1	5.55	123.30	118.30
1	U	213	LEU	N-CA-C	-5.54	96.04	111.00
1	D	213	LEU	N-CA-C	-5.53	96.08	111.00
1	B	213	LEU	N-CA-C	-5.51	96.13	111.00
1	Q	213	LEU	N-CA-C	-5.49	96.19	111.00
1	M	213	LEU	N-CA-C	-5.45	96.29	111.00
1	W	213	LEU	N-CA-C	-5.43	96.34	111.00
1	A	213	LEU	N-CA-C	-5.43	96.34	111.00
1	O	213	LEU	N-CA-C	-5.43	96.34	111.00
1	1	213	LEU	N-CA-C	-5.39	96.44	111.00
1	U	76	ARG	NE-CZ-NH2	-5.39	117.61	120.30
2	N	338	ASP	CB-CG-OD1	5.33	123.10	118.30
2	R	538	HIS	N-CA-C	-5.33	96.61	111.00
1	S	76	ARG	NE-CZ-NH2	-5.32	117.64	120.30
1	S	213	LEU	N-CA-C	-5.25	96.83	111.00
2	C	357	ARG	NE-CZ-NH2	-5.25	117.68	120.30
1	F	76	ARG	NE-CZ-NH2	-5.18	117.71	120.30
2	V	530	ASP	CB-CG-OD2	5.18	122.96	118.30
2	R	530	ASP	CB-CG-OD2	5.15	122.93	118.30
1	I	97	ARG	NE-CZ-NH2	-5.13	117.74	120.30
2	T	338	ASP	CB-CG-OD1	5.12	122.91	118.30
1	F	213	LEU	N-CA-C	-5.11	97.20	111.00
1	U	85	ARG	NE-CZ-NH2	-5.08	117.76	120.30
1	I	76	ARG	NE-CZ-NH2	-5.05	117.77	120.30
1	I	85	ARG	NE-CZ-NH2	-5.02	117.79	120.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	1658	0	1659	55	0
1	A	1654	0	1651	68	0
1	B	1643	0	1639	82	0
1	D	1650	0	1648	99	0
1	F	1699	0	1696	70	0
1	I	1669	0	1668	96	0
1	K	1666	0	1670	67	0
1	M	1666	0	1670	78	0
1	O	1666	0	1670	67	0
1	Q	1658	0	1659	82	0
1	S	1665	0	1668	86	0
1	U	1662	0	1662	51	0
1	W	1669	0	1668	70	0
1	Y	1666	0	1670	80	0
2	2	1642	0	1632	39	0
2	C	1638	0	1629	33	0
2	E	1642	0	1632	47	0
2	G	1638	0	1629	43	0
2	H	1638	0	1629	33	0
2	J	1638	0	1629	43	0
2	L	1642	0	1632	31	0
2	N	1638	0	1629	44	0
2	P	1638	0	1629	31	0
2	R	1767	0	1729	46	0
2	T	1642	0	1632	21	0
2	V	1767	0	1729	40	0
2	X	1642	0	1632	25	0
2	Z	1642	0	1632	26	0
3	1	5	0	7	0	0
3	2	40	0	56	27	0
3	A	10	0	14	1	0
3	B	10	0	14	2	0
3	C	35	0	49	15	0
3	D	25	0	35	6	0
3	E	30	0	42	16	0
3	F	15	0	21	1	0
3	G	45	0	63	31	0
3	H	30	0	42	12	0
3	I	10	0	14	2	0
3	J	15	0	21	7	0
3	K	20	0	28	11	0
3	L	20	0	28	5	0
3	M	20	0	28	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	N	25	0	35	26	0
3	O	15	0	21	1	0
3	P	40	0	56	14	0
3	Q	15	0	21	9	0
3	R	25	0	35	13	0
3	S	10	0	14	1	0
3	T	30	0	42	15	0
3	U	10	0	14	8	0
3	V	45	0	63	48	0
3	W	10	0	14	7	0
3	X	25	0	35	7	0
3	Y	15	0	21	4	0
3	Z	20	0	28	8	0
4	2	20	0	22	4	0
4	C	20	0	22	3	0
4	E	20	0	22	3	0
4	G	20	0	22	3	0
4	H	20	0	22	5	0
4	J	20	0	22	2	0
4	L	20	0	22	3	0
4	N	20	0	22	3	0
4	P	20	0	22	4	0
4	R	20	0	22	3	0
4	T	20	0	22	3	0
4	V	20	0	22	4	0
4	X	20	0	22	4	0
4	Z	20	0	22	3	0
5	1	47	0	0	1	0
5	2	143	0	0	7	0
5	A	43	0	0	4	0
5	B	41	0	0	6	0
5	C	163	0	0	10	0
5	D	40	0	0	8	0
5	E	166	0	0	9	0
5	F	58	0	0	5	0
5	G	131	0	0	2	0
5	H	148	0	0	7	0
5	I	52	0	0	10	0
5	J	142	0	0	10	0
5	K	45	0	0	5	0
5	L	153	0	0	12	0
5	M	40	0	0	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	N	154	0	0	5	0
5	O	47	0	0	5	0
5	P	139	0	0	6	0
5	Q	38	0	0	9	0
5	R	170	0	0	7	0
5	S	42	0	0	8	0
5	T	116	0	0	7	0
5	U	49	0	0	4	0
5	V	177	0	0	14	0
5	W	35	0	0	4	0
5	X	150	0	0	7	0
5	Y	28	0	0	6	0
5	Z	123	0	0	4	0
All	All	50080	0	47491	1521	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 16.

All (1521) 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:B:7:ILE:HG21	1:B:11:GLN:CG	1.63	1.27
1:F:7:ILE:CG2	1:F:11:GLN:HB3	1.65	1.27
3:R:92:DMF:H21	5:R:1869:HOH:O	1.30	1.23
1:O:9:PRO:HD2	1:U:15:GLU:CG	1.69	1.21
1:A:80:GLN:HE21	1:A:80:GLN:C	1.45	1.20
1:D:8:SER:HB3	1:D:9:PRO:CD	1.73	1.19
1:D:207:SER:O	1:D:208:LEU:HD23	1.41	1.17
3:N:90:DMF:C2	3:V:120:DMF:H11	1.73	1.17
1:Y:7:ILE:HG13	1:Y:8:SER:N	1.52	1.15
3:N:90:DMF:H22	3:V:120:DMF:H11	1.18	1.15
1:Y:13:MET:CE	1:Y:111:PHE:HE2	1.61	1.13
3:U:250:DMF:H23	3:V:27:DMF:H12	1.27	1.13
1:Y:7:ILE:HG13	1:Y:8:SER:H	0.96	1.13
1:B:7:ILE:CG2	1:B:11:GLN:HG2	1.78	1.12
2:Z:456:GLN:NE2	2:Z:465:ARG:HH22	1.48	1.11
2:N:432:GLU:OE1	3:N:104:DMF:H12	1.47	1.11
1:O:9:PRO:HD2	1:U:15:GLU:HG2	1.16	1.10
3:V:83:DMF:H11	5:V:1742:HOH:O	1.51	1.10
1:D:152:HIS:HB3	1:D:171:TYR:CE1	1.88	1.09
1:B:7:ILE:HG21	1:B:11:GLN:HG2	1.22	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:434:GLU:HB2	3:2:4:DMF:H23	1.35	1.06
3:G:12:DMF:H11	5:G:2627:HOH:O	1.53	1.06
2:E:461:ASP:HB2	5:E:1924:HOH:O	1.55	1.05
1:Q:7:ILE:CG2	1:Q:11:GLN:CB	2.35	1.05
1:I:203:LEU:HB3	1:I:207:SER:OG	1.57	1.05
1:Y:13:MET:HE1	1:Y:111:PHE:HE2	1.19	1.04
1:D:174:ASN:N	1:D:174:ASN:HD22	1.55	1.03
3:U:250:DMF:H23	3:V:27:DMF:C1	1.89	1.02
2:P:452:LYS:HB3	3:P:33:DMF:H22	1.40	1.02
1:Q:7:ILE:CG2	1:Q:11:GLN:HB2	1.90	1.01
2:G:447:LYS:HD2	3:G:119:DMF:H23	1.43	1.01
1:D:8:SER:HB3	1:D:9:PRO:HD2	1.42	1.00
2:N:432:GLU:OE2	3:N:104:DMF:H23	1.62	0.99
1:Y:7:ILE:CG1	1:Y:8:SER:H	1.72	0.99
2:H:483:GLY:HA3	3:H:91:DMF:H22	1.44	0.99
1:K:15:GLU:HG2	1:M:9:PRO:HD2	1.42	0.99
3:N:90:DMF:H22	3:V:120:DMF:C1	1.92	0.98
1:D:8:SER:CB	1:D:9:PRO:HD3	1.94	0.97
3:N:22:DMF:HC	5:N:2569:HOH:O	1.64	0.97
1:B:7:ILE:N	1:B:7:ILE:HD12	1.78	0.97
2:N:429:TRP:CZ2	3:N:93:DMF:HC	1.98	0.97
1:A:161:GLU:HB2	1:A:162:PRO:HD3	1.47	0.97
3:C:103:DMF:H11	5:C:1438:HOH:O	1.64	0.97
5:P:223:HOH:O	3:V:82:DMF:HC	1.65	0.97
1:D:185:VAL:HG21	1:D:234:LEU:HD11	1.45	0.97
1:Q:7:ILE:HG22	1:Q:11:GLN:HB2	1.44	0.97
1:Q:161:GLU:HB2	1:Q:162:PRO:HD3	1.46	0.97
1:D:8:SER:CB	1:D:9:PRO:CD	2.40	0.96
1:I:15:GLU:HG3	1:S:9:PRO:HB2	1.47	0.96
1:S:161:GLU:HB2	1:S:162:PRO:HD3	1.48	0.96
3:N:90:DMF:C2	3:V:120:DMF:C1	2.43	0.96
1:W:161:GLU:HB2	1:W:162:PRO:HD3	1.48	0.95
1:Q:8:SER:HB3	1:Y:15:GLU:OE2	1.67	0.95
1:I:10:GLU:O	1:I:14:ARG:HG3	1.66	0.95
1:O:161:GLU:HB2	1:O:162:PRO:HD3	1.49	0.95
1:1:161:GLU:HB2	1:1:162:PRO:HD3	1.49	0.95
1:Q:7:ILE:CG2	1:Q:11:GLN:HB3	1.97	0.95
1:Y:13:MET:CE	1:Y:111:PHE:CE2	2.50	0.95
2:G:447:LYS:HD2	3:G:119:DMF:C2	1.95	0.95
2:T:362:GLU:OE2	2:T:382:ARG:HD3	1.67	0.94
1:M:161:GLU:HB2	1:M:162:PRO:HD3	1.48	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:161:GLU:HB2	1:U:162:PRO:HD3	1.49	0.94
2:E:456:GLN:HE21	2:E:465:ARG:NH2	1.66	0.94
1:K:161:GLU:HB2	1:K:162:PRO:HD3	1.49	0.94
1:Y:161:GLU:HB2	1:Y:162:PRO:HD3	1.49	0.94
1:D:161:GLU:HB2	1:D:162:PRO:HD3	1.48	0.94
1:F:9:PRO:HG2	1:M:15:GLU:HG3	1.48	0.94
1:F:7:ILE:HG22	1:F:11:GLN:HB3	1.46	0.93
1:B:7:ILE:CG2	1:B:11:GLN:CG	2.41	0.93
3:C:103:DMF:H13	2:H:447:LYS:NZ	1.83	0.93
1:B:161:GLU:HB2	1:B:162:PRO:HD3	1.51	0.93
2:E:456:GLN:HE21	2:E:465:ARG:HH21	1.12	0.93
1:A:166:ALA:O	1:A:169:GLU:HG2	1.68	0.93
1:F:161:GLU:HB2	1:F:162:PRO:HD3	1.49	0.93
2:E:436:TYR:CE1	3:E:75:DMF:H22	2.03	0.92
3:U:250:DMF:H12	3:V:27:DMF:H11	1.51	0.92
2:Z:456:GLN:HE21	2:Z:465:ARG:NH2	1.67	0.92
1:I:161:GLU:HB2	1:I:162:PRO:HD3	1.50	0.91
2:J:515:ARG:HH22	2:R:539:HIS:HB2	1.35	0.91
1:Y:13:MET:HE1	1:Y:111:PHE:CE2	2.04	0.91
1:D:15:GLU:HG3	1:K:9:PRO:HG2	1.51	0.91
1:F:7:ILE:CG2	1:F:11:GLN:CB	2.49	0.90
1:I:44:GLU:HG3	1:I:203:LEU:HD21	1.52	0.90
2:N:307:LYS:HD2	2:V:530:ASP:OD1	1.70	0.90
3:W:250:DMF:H23	3:X:16:DMF:H23	1.51	0.90
2:2:434:GLU:CB	3:2:4:DMF:H23	2.00	0.90
1:D:8:SER:HB3	1:D:9:PRO:HD3	1.50	0.90
2:P:472:TYR:CE1	3:P:14:DMF:H12	2.07	0.90
2:Z:456:GLN:HE21	2:Z:465:ARG:HH22	0.94	0.90
2:G:445:PHE:CD2	3:G:64:DMF:H12	2.07	0.89
1:K:7:ILE:HG23	1:K:11:GLN:HB3	1.54	0.89
2:N:362:GLU:OE2	2:N:382:ARG:HD3	1.71	0.89
1:F:7:ILE:HG21	1:F:11:GLN:HB3	1.52	0.89
1:O:9:PRO:CD	1:U:15:GLU:HG2	2.01	0.89
1:W:30:VAL:HG13	1:W:43:ALA:HB2	1.55	0.89
2:G:447:LYS:CD	3:G:119:DMF:H23	2.03	0.89
1:Y:7:ILE:CG1	1:Y:8:SER:N	2.30	0.89
3:G:111:DMF:HC	5:2:807:HOH:O	1.73	0.89
1:B:15:GLU:HG3	1:I:9:PRO:HG2	1.55	0.88
2:H:456:GLN:NE2	2:H:465:ARG:HH21	1.72	0.88
1:D:225:ILE:HA	5:D:2295:HOH:O	1.72	0.87
1:S:152:HIS:HE1	1:S:173:GLU:OE2	1.56	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:186:ALA:O	1:K:189:ARG:HG2	1.75	0.87
1:B:233:LEU:HD12	1:B:233:LEU:N	1.89	0.86
2:2:465:ARG:HH11	2:2:465:ARG:HG3	1.37	0.86
2:E:456:GLN:NE2	2:E:465:ARG:HH21	1.74	0.86
1:O:9:PRO:HD2	1:U:15:GLU:HG3	1.56	0.86
2:R:456:GLN:HE21	2:R:465:ARG:HH21	1.24	0.86
1:B:7:ILE:CG2	1:B:11:GLN:HB3	2.05	0.86
2:J:456:GLN:NE2	2:J:465:ARG:HH21	1.73	0.86
3:T:113:DMF:H11	3:2:112:DMF:O	1.76	0.86
2:J:515:ARG:NH2	2:R:539:HIS:HB2	1.91	0.85
1:B:206:ALA:O	1:B:207:SER:OG	1.93	0.85
1:D:170:SER:HB2	1:D:183:ILE:HG23	1.56	0.85
1:1:30:VAL:HG13	1:1:43:ALA:HB2	1.58	0.85
2:J:515:ARG:NH1	2:R:539:HIS:H	1.74	0.85
2:E:381:ASN:HB2	3:E:53:DMF:H13	1.58	0.85
2:E:521:ARG:HD3	3:E:100:DMF:H12	1.58	0.85
2:N:456:GLN:HE21	2:N:465:ARG:HH21	1.18	0.85
1:O:189:ARG:CG	1:O:203:LEU:CD2	2.55	0.84
2:N:456:GLN:NE2	2:N:465:ARG:HH21	1.75	0.84
2:P:456:GLN:NE2	2:P:465:ARG:HH21	1.74	0.84
2:H:456:GLN:HE21	2:H:465:ARG:HH21	1.23	0.84
5:L:1466:HOH:O	3:P:33:DMF:HC	1.77	0.84
3:U:250:DMF:C2	3:V:27:DMF:C1	2.55	0.84
1:A:182:ARG:HH12	1:A:234:LEU:C	1.79	0.84
1:I:203:LEU:HB3	1:I:207:SER:HG	1.36	0.84
1:Y:25:ALA:O	1:Y:158:GLY:HA2	1.77	0.84
2:C:456:GLN:NE2	2:C:465:ARG:HH21	1.75	0.84
3:E:20:DMF:H21	5:E:2349:HOH:O	1.78	0.84
1:A:80:GLN:NE2	1:A:80:GLN:C	2.30	0.84
1:M:230:LEU:O	1:M:234:LEU:HD22	1.78	0.83
3:T:113:DMF:H11	3:2:112:DMF:C	2.08	0.83
1:U:163:ILE:HG23	1:U:187:ALA:O	1.79	0.83
3:V:83:DMF:H13	3:2:4:DMF:HC	1.58	0.83
1:B:15:GLU:CG	1:I:9:PRO:HG2	2.08	0.83
1:Y:10:GLU:OE1	1:Y:10:GLU:HA	1.79	0.83
1:B:7:ILE:CG2	1:B:11:GLN:CB	2.56	0.82
1:D:182:ARG:HD2	1:D:234:LEU:HD23	1.60	0.82
2:P:452:LYS:HB3	3:P:33:DMF:C2	2.07	0.82
1:D:152:HIS:HB3	1:D:171:TYR:CZ	2.13	0.82
1:S:142:THR:OG1	1:S:146:SER:HB2	1.80	0.82
1:A:27:ALA:HB1	5:A:1907:HOH:O	1.78	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:V:83:DMF:C1	3:2:4:DMF:HC	2.09	0.82
1:D:109:THR:N	3:D:251:DMF:H22	1.95	0.82
1:I:102:VAL:HG12	3:I:250:DMF:H12	1.62	0.82
1:Q:7:ILE:HG23	1:Q:11:GLN:CB	2.10	0.82
1:Q:226:THR:HG22	5:Q:959:HOH:O	1.79	0.81
1:Q:13:MET:HG3	1:Y:19:LEU:HD11	1.61	0.81
1:D:25:ALA:O	1:D:158:GLY:HA2	1.81	0.81
2:C:456:GLN:HE21	2:C:465:ARG:HH21	1.27	0.81
1:I:217:ARG:NH1	1:I:223:ARG:HD3	1.94	0.81
2:G:447:LYS:CD	3:G:119:DMF:C2	2.58	0.80
1:I:15:GLU:HG2	1:S:9:PRO:HD2	1.64	0.80
2:E:472:TYR:CE1	3:E:20:DMF:H12	2.16	0.80
2:P:444:LEU:HB3	5:P:926:HOH:O	1.80	0.80
2:R:445:PHE:CD2	3:R:59:DMF:H12	2.16	0.79
2:R:456:GLN:NE2	2:R:465:ARG:HH21	1.80	0.79
3:W:250:DMF:C2	5:X:2517:HOH:O	2.30	0.79
2:E:521:ARG:HD3	3:E:100:DMF:C1	2.13	0.79
1:1:25:ALA:O	1:1:158:GLY:HA2	1.82	0.79
2:L:432:GLU:HG3	5:L:2512:HOH:O	1.82	0.79
1:B:7:ILE:HG22	1:B:11:GLN:HB3	1.61	0.79
2:X:496:ILE:HG21	3:X:40:DMF:H13	1.63	0.79
2:N:432:GLU:OE1	3:N:104:DMF:C1	2.29	0.79
1:B:7:ILE:HG21	1:B:11:GLN:CB	2.13	0.78
2:J:396:GLN:OE1	2:J:396:GLN:HA	1.80	0.78
3:C:103:DMF:C	3:H:43:DMF:H22	2.13	0.78
2:E:324:ASN:HB2	5:E:2164:HOH:O	1.82	0.78
1:B:15:GLU:HG2	1:I:9:PRO:HD2	1.64	0.78
2:N:430:ASN:HB2	5:N:2370:HOH:O	1.83	0.78
1:A:15:GLU:HB3	1:B:9:PRO:HG2	1.66	0.78
3:C:103:DMF:H13	2:H:447:LYS:HZ2	1.46	0.77
2:L:362:GLU:OE2	2:L:382:ARG:HD3	1.84	0.77
1:S:152:HIS:CE1	1:S:173:GLU:OE2	2.37	0.77
2:N:388:ARG:HD3	2:N:426:ALA:O	1.84	0.77
1:S:15:GLU:HG3	1:1:9:PRO:HD2	1.65	0.77
2:G:430:ASN:ND2	3:G:98:DMF:C	2.48	0.77
1:W:74:LEU:HD23	1:W:122:LEU:HD11	1.66	0.77
2:J:456:GLN:HE21	2:J:465:ARG:HH21	1.29	0.77
1:D:173:GLU:HB3	1:D:174:ASN:ND2	1.99	0.77
2:T:335:TYR:HB3	3:T:29:DMF:H13	1.66	0.77
2:G:456:GLN:NE2	2:G:465:ARG:HH21	1.83	0.77
2:2:509:ARG:HH12	3:2:52:DMF:C	1.97	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:230:LEU:O	1:A:234:LEU:HD22	1.84	0.77
1:B:22:LYS:HD2	1:I:10:GLU:OE2	1.84	0.77
1:Q:181:LEU:HD23	1:Q:233:LEU:HB3	1.66	0.77
2:T:362:GLU:OE2	2:T:382:ARG:CD	2.32	0.76
2:E:456:GLN:NE2	2:E:465:ARG:NH2	2.30	0.76
1:W:142:THR:OG1	1:W:146:SER:HB2	1.86	0.76
1:I:110:ILE:HG23	1:I:114:GLN:HG3	1.68	0.76
1:M:231:GLN:O	1:M:234:LEU:HD23	1.84	0.76
2:E:508:SER:OG	3:E:73:DMF:H13	1.86	0.75
1:D:207:SER:O	1:D:208:LEU:CD2	2.30	0.75
2:L:362:GLU:OE2	2:L:382:ARG:CD	2.35	0.75
1:O:189:ARG:CG	1:O:203:LEU:HD21	2.16	0.75
1:O:189:ARG:HG3	1:O:203:LEU:CD2	2.17	0.75
2:P:456:GLN:HE21	2:P:465:ARG:HH21	1.32	0.75
2:Z:483:GLY:HA3	3:Z:18:DMF:H22	1.67	0.75
2:V:429:TRP:CH2	3:V:42:DMF:H13	2.22	0.74
2:N:477:ASP:OD1	3:N:118:DMF:H12	1.88	0.74
2:V:483:GLY:HA3	3:V:116:DMF:H23	1.69	0.74
1:Y:30:VAL:HG13	1:Y:43:ALA:HB2	1.69	0.74
2:G:361:VAL:HG12	3:G:62:DMF:HC	1.70	0.74
3:U:250:DMF:C1	3:V:27:DMF:H11	2.17	0.74
1:I:97:ARG:CZ	5:I:2433:HOH:O	2.36	0.74
1:M:87:TYR:O	2:N:357:ARG:NH1	2.20	0.74
2:P:456:GLN:HE21	2:P:465:ARG:NH2	1.86	0.74
1:Y:181:LEU:HD23	1:Y:233:LEU:HG	1.69	0.73
2:C:388:ARG:HD3	2:C:426:ALA:O	1.88	0.73
2:J:456:GLN:HE21	2:J:465:ARG:NH2	1.85	0.73
1:F:7:ILE:HD11	1:W:8:SER:HB2	1.70	0.73
5:Q:2679:HOH:O	3:Z:54:DMF:C	2.36	0.73
1:D:209:GLU:HA	5:D:2415:HOH:O	1.89	0.73
1:D:217:ARG:HG2	1:D:220:ARG:O	1.88	0.73
1:F:7:ILE:HG21	1:F:11:GLN:CB	2.14	0.73
1:M:25:ALA:O	1:M:158:GLY:HA2	1.88	0.73
2:T:326:ILE:O	3:T:115:DMF:H21	1.88	0.73
2:E:434:GLU:HB3	3:E:75:DMF:H21	1.70	0.73
1:F:170:SER:OG	1:F:183:ILE:HG23	1.88	0.73
3:W:250:DMF:H22	5:X:2517:HOH:O	1.89	0.73
1:F:7:ILE:HG21	1:F:11:GLN:CG	2.19	0.73
2:H:456:GLN:HE21	2:H:465:ARG:NH2	1.86	0.73
2:H:335:TYR:CE1	3:H:66:DMF:HC	2.24	0.73
2:J:388:ARG:HD3	2:J:426:ALA:O	1.88	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:30:VAL:HG13	1:D:43:ALA:HB2	1.70	0.72
1:B:7:ILE:HG22	1:B:11:GLN:CB	2.18	0.72
2:C:301:THR:N	4:C:300:SA6:HO6	1.88	0.72
2:N:362:GLU:OE2	2:N:382:ARG:CD	2.36	0.72
1:B:41:PHE:HB3	1:B:53:ILE:HD13	1.70	0.72
1:B:223:ARG:HG2	5:B:2211:HOH:O	1.90	0.72
2:E:357:ARG:HA	3:E:28:DMF:HC	1.71	0.72
5:Q:2679:HOH:O	3:Z:54:DMF:HC	1.87	0.72
2:N:456:GLN:HE21	2:N:465:ARG:NH2	1.87	0.72
1:Y:10:GLU:CA	1:Y:10:GLU:OE1	2.37	0.72
1:I:203:LEU:HD23	1:I:207:SER:HB2	1.70	0.72
1:Q:13:MET:SD	3:Q:250:DMF:C1	2.78	0.72
1:K:25:ALA:O	1:K:158:GLY:HA2	1.89	0.72
1:S:30:VAL:HG13	1:S:43:ALA:HB2	1.72	0.72
1:W:185:VAL:HG12	1:W:189:ARG:NH2	2.03	0.72
2:C:456:GLN:HE21	2:C:465:ARG:NH2	1.87	0.71
1:D:8:SER:OG	1:D:9:PRO:HD3	1.89	0.71
1:Q:25:ALA:O	1:Q:158:GLY:HA2	1.90	0.71
1:I:15:GLU:CG	1:S:9:PRO:HB2	2.20	0.71
1:Q:7:ILE:HG22	1:Q:8:SER:N	2.04	0.71
1:S:97:ARG:NH2	5:S:1917:HOH:O	2.23	0.71
1:W:25:ALA:O	1:W:158:GLY:HA2	1.89	0.71
2:X:301:THR:N	4:X:300:SA6:HO6	1.88	0.71
1:D:174:ASN:N	1:D:174:ASN:ND2	2.30	0.71
1:K:30:VAL:HG13	1:K:43:ALA:HB2	1.72	0.71
1:S:15:GLU:CD	1:I:8:SER:HB3	2.10	0.71
1:S:8:SER:H	1:S:11:GLN:HB2	1.55	0.71
1:Y:214:ASP:OD1	1:Y:216:ASN:N	2.22	0.71
3:K:250:DMF:H11	5:L:1474:HOH:O	1.91	0.71
2:V:388:ARG:HD3	2:V:426:ALA:O	1.90	0.71
1:O:30:VAL:HG13	1:O:43:ALA:HB2	1.73	0.71
3:T:113:DMF:C1	3:2:112:DMF:O	2.39	0.71
1:U:30:VAL:HG13	1:U:43:ALA:HB2	1.72	0.71
2:H:335:TYR:CE1	3:H:66:DMF:C	2.74	0.71
1:M:189:ARG:NH1	1:M:203:LEU:N	2.38	0.71
2:2:331:VAL:HG11	4:2:300:SA6:H19	1.73	0.70
2:T:388:ARG:HD3	2:T:426:ALA:O	1.90	0.70
2:V:434:GLU:HB2	3:V:32:DMF:C2	2.21	0.70
1:D:105:GLN:HB2	5:D:1313:HOH:O	1.91	0.70
1:F:25:ALA:O	1:F:158:GLY:HA2	1.92	0.70
1:Y:13:MET:HE3	1:Y:111:PHE:CE2	2.27	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:484:PRO:HD2	5:E:2667:HOH:O	1.90	0.70
2:J:465:ARG:HD2	3:J:123:DMF:HC	1.74	0.70
3:V:83:DMF:H22	2:2:447:LYS:NZ	2.07	0.70
1:Y:121:GLU:HG3	5:Y:2504:HOH:O	1.91	0.70
1:B:105:GLN:HB2	5:B:1751:HOH:O	1.92	0.70
1:U:41:PHE:HB3	1:U:53:ILE:HD13	1.73	0.70
2:Z:409:ILE:HG12	5:Z:1615:HOH:O	1.91	0.70
1:B:7:ILE:HG21	1:B:11:GLN:HG3	1.70	0.70
1:Y:92:ARG:NH1	5:Y:1747:HOH:O	2.24	0.70
1:A:25:ALA:O	1:A:158:GLY:HA2	1.91	0.69
1:F:9:PRO:CG	1:M:15:GLU:HG3	2.20	0.69
1:B:19:LEU:O	1:B:19:LEU:HD23	1.91	0.69
1:A:15:GLU:HB3	1:B:9:PRO:CG	2.21	0.69
1:M:41:PHE:HB3	1:M:53:ILE:HD13	1.74	0.69
1:1:189:ARG:HH12	1:1:203:LEU:N	1.89	0.69
1:Q:7:ILE:HG21	1:Q:11:GLN:HB3	1.74	0.69
2:E:466:VAL:HG23	5:E:2061:HOH:O	1.93	0.69
1:Q:21:ARG:HD2	5:Q:2238:HOH:O	1.93	0.69
1:Y:10:GLU:O	1:Y:10:GLU:CD	2.30	0.69
1:A:30:VAL:HG13	1:A:43:ALA:HB2	1.75	0.69
1:D:8:SER:HB2	1:Q:7:ILE:HG13	1.72	0.69
2:Z:519:GLU:HG3	5:Z:1992:HOH:O	1.92	0.69
1:B:30:VAL:HG13	1:B:43:ALA:HB2	1.73	0.69
1:I:226:THR:HG22	5:I:691:HOH:O	1.90	0.69
1:1:11:GLN:HA	1:1:11:GLN:HE21	1.58	0.69
1:1:170:SER:HB2	1:1:183:ILE:HG23	1.73	0.69
1:B:233:LEU:HD12	1:B:233:LEU:H	1.57	0.69
2:R:332:ARG:HD3	5:R:1572:HOH:O	1.92	0.69
2:G:388:ARG:HD3	2:G:426:ALA:O	1.93	0.69
1:I:30:VAL:HG13	1:I:43:ALA:HB2	1.75	0.69
2:J:398:LEU:HD12	2:J:398:LEU:N	2.08	0.69
1:U:110:ILE:HG23	1:U:114:GLN:NE2	2.08	0.69
2:Z:456:GLN:NE2	2:Z:465:ARG:NH2	2.30	0.68
1:M:31:VAL:HG12	1:M:155:VAL:HG22	1.75	0.68
1:A:182:ARG:NH1	1:A:234:LEU:HA	2.08	0.68
3:V:83:DMF:H22	2:2:447:LYS:HZ2	1.59	0.68
1:Q:31:VAL:HG12	1:Q:155:VAL:HG22	1.75	0.68
1:W:185:VAL:CG1	1:W:189:ARG:NH2	2.57	0.68
1:W:77:GLY:HA3	3:W:249:DMF:H12	1.75	0.68
1:1:31:VAL:HG12	1:1:155:VAL:HG22	1.75	0.68
2:R:445:PHE:CD2	3:R:59:DMF:C1	2.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:31:VAL:HG12	1:Y:155:VAL:HG22	1.75	0.68
1:D:152:HIS:CG	1:D:171:TYR:CZ	2.82	0.68
1:K:114:GLN:OE1	3:K:252:DMF:C1	2.41	0.68
1:K:41:PHE:HB3	1:K:53:ILE:HD13	1.74	0.68
2:P:447:LYS:HD2	3:P:107:DMF:H23	1.76	0.68
2:X:331:VAL:HG11	4:X:300:SA6:H19	1.76	0.68
1:D:182:ARG:HD2	1:D:234:LEU:CD2	2.22	0.68
1:W:31:VAL:HG12	1:W:155:VAL:HG22	1.75	0.68
1:A:163:ILE:CG2	1:A:187:ALA:HB1	2.24	0.68
1:A:182:ARG:NH1	1:A:234:LEU:C	2.47	0.68
1:D:173:GLU:C	1:D:174:ASN:HD22	1.97	0.68
2:E:388:ARG:HD3	2:E:426:ALA:O	1.94	0.68
2:J:456:GLN:NE2	2:J:465:ARG:NH2	2.42	0.68
1:W:41:PHE:HB3	1:W:53:ILE:HD13	1.76	0.68
3:C:103:DMF:C1	2:H:447:LYS:NZ	2.57	0.67
1:Q:7:ILE:HG23	1:Q:11:GLN:HB3	1.71	0.67
2:X:456:GLN:NE2	2:X:465:ARG:HH21	1.92	0.67
1:F:30:VAL:HG13	1:F:43:ALA:HB2	1.76	0.67
1:Y:41:PHE:HB3	1:Y:53:ILE:HD13	1.77	0.67
1:F:8:SER:HB2	1:M:15:GLU:HG2	1.77	0.67
1:K:97:ARG:NH1	5:K:1987:HOH:O	2.28	0.67
2:P:456:GLN:NE2	2:P:465:ARG:NH2	2.42	0.67
2:X:456:GLN:HE21	2:X:465:ARG:HH21	1.41	0.67
1:O:173:GLU:HG2	1:O:174:ASN:OD1	1.94	0.67
3:C:103:DMF:C1	2:H:447:LYS:HZ2	2.07	0.67
2:R:456:GLN:HE21	2:R:465:ARG:NH2	1.91	0.67
1:U:142:THR:OG1	1:U:146:SER:HB2	1.94	0.67
2:H:388:ARG:HD3	2:H:426:ALA:O	1.95	0.67
1:U:9:PRO:HG2	1:1:15:GLU:HG3	1.76	0.67
1:Y:165:ASN:O	1:Y:169:GLU:HG2	1.95	0.67
1:K:7:ILE:CG1	1:K:11:GLN:HG2	2.25	0.67
1:S:31:VAL:HG12	1:S:155:VAL:HG22	1.75	0.67
1:D:11:GLN:O	1:D:15:GLU:HB2	1.94	0.66
3:K:250:DMF:C1	5:L:1474:HOH:O	2.43	0.66
1:D:31:VAL:HG12	1:D:155:VAL:HG22	1.76	0.66
2:L:461:ASP:OD1	2:L:509:ARG:NH1	2.28	0.66
2:N:301:THR:N	4:N:300:SA6:HO6	1.93	0.66
2:R:388:ARG:HD3	2:R:426:ALA:O	1.93	0.66
1:A:185:VAL:O	1:A:189:ARG:HG3	1.94	0.66
2:E:301:THR:N	4:E:300:SA6:HO6	1.93	0.66
2:V:434:GLU:HB2	3:V:32:DMF:H22	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:980:HOH:O	1:K:112:THR:HG21	1.96	0.66
2:T:301:THR:N	4:T:300:SA6:HO6	1.93	0.66
2:Z:429:TRP:CH2	3:Z:54:DMF:H22	2.31	0.66
1:I:15:GLU:HG2	1:S:9:PRO:CD	2.26	0.66
1:O:189:ARG:HG3	1:O:203:LEU:HD21	1.75	0.66
1:Q:41:PHE:HB3	1:Q:53:ILE:HD13	1.76	0.66
1:U:31:VAL:HG12	1:U:155:VAL:HG22	1.75	0.66
2:G:472:TYR:CE1	3:G:12:DMF:H22	2.30	0.66
2:H:515:ARG:HD2	5:H:542:HOH:O	1.94	0.66
1:K:219:ARG:CZ	3:K:250:DMF:H21	2.25	0.66
1:I:47:SER:HB2	5:S:1142:HOH:O	1.96	0.66
2:V:331:VAL:HG11	4:V:300:SA6:H19	1.76	0.66
2:L:331:VAL:HG11	4:L:300:SA6:H19	1.76	0.66
1:A:163:ILE:HG23	1:A:187:ALA:C	2.17	0.66
2:P:331:VAL:HG11	4:P:300:SA6:H19	1.78	0.66
2:P:388:ARG:HD3	2:P:426:ALA:O	1.96	0.66
3:U:250:DMF:C2	3:V:27:DMF:H12	2.12	0.66
1:O:25:ALA:O	1:O:158:GLY:HA2	1.96	0.65
1:O:189:ARG:HG2	1:O:203:LEU:CD2	2.26	0.65
1:S:8:SER:O	1:S:11:GLN:N	2.29	0.65
1:B:15:GLU:CG	1:I:9:PRO:HD2	2.25	0.65
1:B:226:THR:HB	5:B:1186:HOH:O	1.96	0.65
1:K:102:VAL:CG2	3:K:251:DMF:HC	2.26	0.65
1:M:141:ILE:N	1:M:141:ILE:HD12	2.11	0.65
1:B:7:ILE:HG22	1:B:8:SER:H	1.60	0.65
2:P:472:TYR:CD1	3:P:14:DMF:H12	2.31	0.65
1:I:41:PHE:HB3	1:I:53:ILE:HD13	1.79	0.65
2:G:445:PHE:CD2	3:G:64:DMF:C1	2.78	0.65
1:O:189:ARG:HG2	1:O:203:LEU:HD21	1.78	0.65
2:H:301:THR:N	4:H:300:SA6:HO6	1.95	0.65
1:M:30:VAL:HG13	1:M:43:ALA:HB2	1.78	0.65
2:G:436:TYR:O	3:G:119:DMF:H13	1.97	0.65
1:M:111:PHE:CE1	1:M:143:TYR:CE1	2.85	0.65
1:S:31:VAL:HB	5:S:2352:HOH:O	1.96	0.65
1:S:15:GLU:CG	1:I:9:PRO:HD2	2.26	0.65
1:S:165:ASN:O	1:S:169:GLU:HG2	1.97	0.65
1:U:9:PRO:HD2	1:I:15:GLU:HG2	1.77	0.65
1:F:97:ARG:HG2	5:F:2227:HOH:O	1.97	0.65
2:L:465:ARG:HD2	5:L:155:HOH:O	1.97	0.64
1:S:85:ARG:HD3	1:S:89:TYR:CD2	2.33	0.64
1:W:223:ARG:CD	5:W:1767:HOH:O	2.45	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:41:PHE:HB3	1:D:53:ILE:HD13	1.79	0.64
1:U:25:ALA:O	1:U:158:GLY:HA2	1.97	0.64
1:W:28:LYS:HD2	1:W:44:GLU:CD	2.16	0.64
2:Z:301:THR:N	4:Z:300:SA6:HO6	1.95	0.64
1:A:163:ILE:HG23	1:A:187:ALA:HB1	1.80	0.64
2:H:335:TYR:CD1	3:H:66:DMF:HC	2.33	0.64
1:Q:30:VAL:HG13	1:Q:43:ALA:HB2	1.79	0.64
3:V:116:DMF:C	5:V:2127:HOH:O	2.45	0.64
2:X:320:SER:HB3	2:X:331:VAL:HG21	1.80	0.64
1:A:9:PRO:HD2	1:O:15:GLU:HG2	1.79	0.64
1:U:97:ARG:NH2	5:U:1445:HOH:O	2.30	0.64
2:E:331:VAL:HG11	4:E:300:SA6:H19	1.79	0.64
1:A:80:GLN:NE2	1:A:80:GLN:O	2.30	0.64
1:I:8:SER:O	1:I:11:GLN:N	2.30	0.64
2:V:538:HIS:HD2	5:V:1790:HOH:O	1.79	0.64
1:W:223:ARG:HD2	5:W:1767:HOH:O	1.98	0.64
1:B:97:ARG:NH2	5:B:2179:HOH:O	2.30	0.64
2:T:432:GLU:HG3	2:T:437:GLN:HB2	1.79	0.64
1:Y:48:ARG:NH1	5:Y:2550:HOH:O	2.30	0.64
1:B:170:SER:HB3	1:B:183:ILE:HG23	1.80	0.63
1:M:111:PHE:CE1	1:M:143:TYR:CD1	2.86	0.63
1:I:112:THR:HG22	1:I:113:GLU:OE2	1.98	0.63
1:I:97:ARG:NH2	5:I:1706:HOH:O	2.30	0.63
2:J:301:THR:N	4:J:300:SA6:HO6	1.95	0.63
1:S:41:PHE:HB3	1:S:53:ILE:HD13	1.80	0.63
3:N:118:DMF:H22	3:V:32:DMF:C	2.29	0.63
1:Y:181:LEU:HD22	1:Y:233:LEU:HD23	1.79	0.63
2:H:447:LYS:HD2	3:H:43:DMF:H21	1.80	0.63
1:O:41:PHE:HB3	1:O:53:ILE:HD13	1.79	0.63
1:F:41:PHE:HB3	1:F:53:ILE:HD13	1.80	0.63
1:K:7:ILE:HG12	1:K:11:GLN:HG2	1.81	0.63
2:N:382:ARG:NH2	2:N:385:ILE:HD13	2.13	0.63
1:O:14:ARG:HB3	1:O:14:ARG:HH11	1.62	0.63
1:S:15:GLU:HB3	1:I:9:PRO:HG2	1.80	0.63
2:G:301:THR:N	4:G:300:SA6:HO6	1.97	0.63
2:H:483:GLY:HA3	3:H:91:DMF:C2	2.24	0.63
3:U:250:DMF:N	3:V:27:DMF:C1	2.61	0.63
1:F:31:VAL:HG12	1:F:155:VAL:HG22	1.79	0.63
2:2:388:ARG:HD3	2:2:426:ALA:O	1.99	0.63
2:N:429:TRP:CZ2	3:N:93:DMF:C	2.78	0.62
1:S:25:ALA:O	1:S:158:GLY:HA2	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:152:HIS:CB	1:D:171:TYR:CZ	2.81	0.62
2:N:331:VAL:HG11	4:N:300:SA6:H19	1.79	0.62
2:J:516:ALA:HB3	3:J:123:DMF:H12	1.79	0.62
2:L:401:LEU:HD12	3:L:97:DMF:H12	1.82	0.62
1:S:7:ILE:HG22	1:S:11:GLN:HB3	1.82	0.62
1:Q:7:ILE:CG2	1:Q:8:SER:N	2.63	0.62
2:G:456:GLN:NE2	2:G:465:ARG:NH2	2.47	0.62
2:H:331:VAL:HG11	4:H:300:SA6:H19	1.80	0.62
1:A:31:VAL:HG12	1:A:155:VAL:HG22	1.79	0.62
1:I:25:ALA:O	1:I:158:GLY:HA2	1.99	0.62
1:S:185:VAL:O	1:S:189:ARG:HG3	2.00	0.62
3:W:250:DMF:H23	3:X:16:DMF:C2	2.27	0.62
2:G:331:VAL:HG11	4:G:300:SA6:H19	1.82	0.62
2:G:456:GLN:HE21	2:G:465:ARG:NH2	1.98	0.62
1:B:15:GLU:HG3	1:I:9:PRO:CG	2.28	0.62
2:J:320:SER:HB3	2:J:331:VAL:HG21	1.82	0.62
3:K:250:DMF:H13	5:K:1480:HOH:O	1.99	0.62
2:R:444:LEU:H	3:R:59:DMF:C	2.12	0.62
3:N:90:DMF:H21	3:V:120:DMF:H11	1.78	0.62
2:2:419:ARG:HD3	3:2:108:DMF:HC	1.82	0.61
2:C:331:VAL:HG11	4:C:300:SA6:H19	1.82	0.61
1:M:163:ILE:HG23	1:M:187:ALA:O	2.00	0.61
1:B:31:VAL:HG12	1:B:155:VAL:HG22	1.82	0.61
1:Y:52:LYS:HG2	3:Y:251:DMF:HC	1.83	0.61
2:Z:508:SER:O	2:Z:512:GLU:HG3	2.01	0.61
2:N:345:ILE:HB	2:N:352:ALA:HB1	1.83	0.61
2:Z:357:ARG:HD3	5:Z:2331:HOH:O	2.00	0.61
2:2:301:THR:N	4:2:300:SA6:HO6	1.99	0.61
1:I:31:VAL:HG12	1:I:155:VAL:HG22	1.82	0.61
1:O:31:VAL:HG12	1:O:155:VAL:HG22	1.83	0.61
1:U:9:PRO:CG	1:I:15:GLU:HG3	2.30	0.61
1:K:31:VAL:HG12	1:K:155:VAL:HG22	1.81	0.61
1:Q:95:THR:OG1	1:Q:98:GLN:HG3	1.99	0.61
2:R:301:THR:N	4:R:300:SA6:HO6	1.98	0.61
1:B:173:GLU:HG3	1:B:174:ASN:ND2	2.16	0.61
1:F:9:PRO:HD2	1:M:15:GLU:CG	2.31	0.61
1:O:76:ARG:HD3	5:O:1434:HOH:O	2.00	0.61
1:B:25:ALA:O	1:B:158:GLY:HA2	2.00	0.61
1:B:18:GLU:OE1	1:B:21:ARG:NH2	2.30	0.61
2:C:320:SER:HB3	2:C:331:VAL:HG21	1.82	0.61
2:2:320:SER:HB3	2:2:331:VAL:HG21	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:181:LEU:HD23	1:D:233:LEU:HB3	1.82	0.60
1:M:203:LEU:N	1:M:203:LEU:HD23	2.16	0.60
2:T:331:VAL:HG11	4:T:300:SA6:H19	1.83	0.60
1:A:41:PHE:HB3	1:A:53:ILE:HD13	1.83	0.60
2:P:472:TYR:CZ	3:P:14:DMF:H12	2.36	0.60
1:S:169:GLU:HA	1:S:169:GLU:OE1	2.01	0.60
1:Y:185:VAL:O	1:Y:189:ARG:HG3	2.01	0.60
2:2:434:GLU:HB2	3:2:4:DMF:C2	2.21	0.60
2:L:388:ARG:NH1	5:L:2158:HOH:O	2.29	0.60
2:2:366:TYR:CD1	3:2:87:DMF:HC	2.36	0.60
1:A:80:GLN:NE2	5:A:1422:HOH:O	2.30	0.60
2:E:515:ARG:NH1	5:E:2580:HOH:O	2.35	0.60
1:A:182:ARG:NH1	1:A:234:LEU:CA	2.64	0.60
2:Z:320:SER:HB3	2:Z:331:VAL:HG21	1.84	0.60
1:A:77:GLY:HA3	3:A:249:DMF:C	2.32	0.60
3:R:95:DMF:HC	5:R:267:HOH:O	2.00	0.60
1:S:15:GLU:OE1	1:1:8:SER:HB3	2.00	0.60
1:M:112:THR:HG22	1:M:113:GLU:OE2	2.02	0.60
2:R:320:SER:HB3	2:R:331:VAL:HG21	1.82	0.60
1:S:205:VAL:CG2	1:S:205:VAL:O	2.50	0.60
1:Y:163:ILE:HG23	1:Y:187:ALA:O	2.02	0.60
2:2:366:TYR:HD1	3:2:87:DMF:HC	1.65	0.60
1:I:142:THR:OG1	1:I:146:SER:HB2	2.02	0.60
2:V:398:LEU:HD12	2:V:398:LEU:N	2.16	0.60
1:D:112:THR:HG22	1:D:113:GLU:OE2	2.02	0.60
2:H:456:GLN:NE2	2:H:465:ARG:NH2	2.46	0.60
1:Q:11:GLN:O	1:Q:15:GLU:HG2	2.02	0.60
2:V:354:GLU:HG2	3:2:101:DMF:H22	1.84	0.60
1:Y:182:ARG:NH1	1:Y:234:LEU:O	2.35	0.60
1:F:112:THR:HG22	1:F:113:GLU:OE2	2.02	0.59
1:I:11:GLN:O	1:I:15:GLU:HB2	2.02	0.59
2:J:398:LEU:CD1	2:J:398:LEU:N	2.65	0.59
1:K:178:THR:HG22	1:K:182:ARG:HE	1.67	0.59
1:Q:7:ILE:HG23	1:Q:11:GLN:OE1	2.01	0.59
2:V:381:ASN:HB2	3:V:42:DMF:H21	1.84	0.59
1:Y:112:THR:HG22	1:Y:113:GLU:OE2	2.01	0.59
1:O:14:ARG:HB3	1:O:14:ARG:NH1	2.17	0.59
2:P:436:TYR:CE1	3:P:107:DMF:H22	2.36	0.59
1:Q:8:SER:N	1:Q:11:GLN:OE1	2.29	0.59
1:U:112:THR:HG22	1:U:113:GLU:OE2	2.02	0.59
1:B:112:THR:HG22	1:B:113:GLU:OE2	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:432:GLU:CD	3:N:104:DMF:H12	2.21	0.59
1:F:181:LEU:O	1:F:185:VAL:HG23	2.02	0.59
1:I:76:ARG:HD3	5:I:339:HOH:O	2.02	0.59
3:N:22:DMF:H13	5:N:674:HOH:O	2.02	0.59
1:I:41:PHE:HB3	1:I:53:ILE:HD13	1.83	0.59
1:A:9:PRO:HB2	1:O:15:GLU:HG3	1.84	0.59
1:W:112:THR:HG22	1:W:113:GLU:OE2	2.02	0.59
1:D:136:PRO:O	1:Q:48:ARG:NH2	2.35	0.59
1:D:15:GLU:HG3	1:K:9:PRO:CG	2.30	0.59
1:K:102:VAL:HG23	3:K:251:DMF:HC	1.85	0.59
1:M:231:GLN:HA	1:M:234:LEU:HD21	1.83	0.59
1:W:142:THR:HG1	1:W:146:SER:HB2	1.68	0.59
1:A:112:THR:HG22	1:A:113:GLU:OE2	2.02	0.59
1:I:163:ILE:HG23	1:I:187:ALA:O	2.03	0.59
1:A:161:GLU:HB2	1:A:162:PRO:CD	2.29	0.59
1:S:112:THR:HG22	1:S:113:GLU:OE2	2.02	0.59
2:P:476:ASP:OD1	3:P:14:DMF:H22	2.03	0.59
2:G:320:SER:HB3	2:G:331:VAL:HG21	1.85	0.58
1:S:161:GLU:HB2	1:S:162:PRO:CD	2.30	0.58
1:A:112:THR:HG22	1:O:115:ALA:HB3	1.85	0.58
1:I:112:THR:HG22	1:I:113:GLU:OE2	2.03	0.58
1:M:10:GLU:HG3	1:M:11:GLN:N	2.18	0.58
2:P:436:TYR:CE1	3:P:107:DMF:C2	2.87	0.58
1:Q:178:THR:HG22	1:Q:182:ARG:HE	1.67	0.58
1:Q:52:LYS:NZ	5:Q:1538:HOH:O	2.36	0.58
1:D:8:SER:O	1:D:11:GLN:HB3	2.04	0.58
1:W:161:GLU:HB2	1:W:162:PRO:CD	2.31	0.58
1:W:163:ILE:HG23	1:W:187:ALA:O	2.03	0.58
5:X:2666:HOH:O	3:Z:94:DMF:H11	2.04	0.58
2:E:516:ALA:HB3	5:E:1124:HOH:O	2.02	0.58
2:L:362:GLU:OE2	2:L:382:ARG:HD2	2.03	0.58
2:P:320:SER:HB3	2:P:331:VAL:HG21	1.85	0.58
1:A:16:ARG:NH2	1:A:114:GLN:O	2.31	0.58
1:B:178:THR:HG22	1:B:182:ARG:HE	1.69	0.58
1:I:152:HIS:HB3	1:I:171:TYR:CE2	2.39	0.58
1:S:178:THR:HG22	1:S:182:ARG:HE	1.69	0.58
2:E:509:ARG:NH1	2:E:512:GLU:OE1	2.37	0.58
1:K:7:ILE:HG13	1:K:11:GLN:HE21	1.69	0.58
1:U:110:ILE:HG23	1:U:114:GLN:HE21	1.68	0.58
2:C:412:SER:O	2:C:414:PRO:HD3	2.04	0.58
2:Z:488:ARG:NE	3:Z:94:DMF:H22	2.19	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:173:GLU:O	1:I:174:ASN:HB2	2.04	0.57
1:K:112:THR:HG22	1:K:113:GLU:OE2	2.03	0.57
1:M:170:SER:HB2	1:M:183:ILE:HG23	1.85	0.57
1:W:223:ARG:HG2	5:W:2456:HOH:O	2.04	0.57
2:X:456:GLN:HE21	2:X:465:ARG:NH2	2.02	0.57
2:H:391:LEU:HB3	5:H:2626:HOH:O	2.05	0.57
1:I:223:ARG:HG2	5:I:1626:HOH:O	2.02	0.57
2:J:331:VAL:HG11	4:J:300:SA6:H19	1.86	0.57
1:K:114:GLN:OE1	3:K:252:DMF:H11	2.03	0.57
2:R:388:ARG:NH1	5:R:2204:HOH:O	2.36	0.57
3:C:69:DMF:H11	5:C:557:HOH:O	2.04	0.57
1:O:102:VAL:HG12	3:O:250:DMF:H22	1.86	0.57
1:S:85:ARG:HD3	1:S:89:TYR:HD2	1.68	0.57
1:W:76:ARG:NH1	2:X:370:GLU:OE2	2.37	0.57
2:L:401:LEU:HD12	3:L:97:DMF:C1	2.34	0.57
1:S:149:ASP:CB	5:S:1142:HOH:O	2.52	0.57
1:A:163:ILE:HG12	1:A:187:ALA:O	2.05	0.57
2:H:320:SER:HB3	2:H:331:VAL:HG21	1.85	0.57
2:J:465:ARG:NH1	5:J:1886:HOH:O	2.35	0.57
1:M:178:THR:HG22	1:M:182:ARG:HE	1.68	0.57
1:Q:161:GLU:HB2	1:Q:162:PRO:CD	2.29	0.57
1:D:189:ARG:N	5:D:2659:HOH:O	2.35	0.57
2:N:477:ASP:OD1	3:N:118:DMF:C1	2.51	0.57
1:D:84:THR:OG1	3:D:253:DMF:HC	2.05	0.57
1:K:110:ILE:HA	1:K:114:GLN:HG3	1.85	0.57
1:K:15:GLU:HG2	1:M:9:PRO:CD	2.25	0.57
2:V:301:THR:N	4:V:300:SA6:HO6	2.02	0.57
2:G:442:GLY:C	3:G:64:DMF:H11	2.24	0.57
2:H:412:SER:O	2:H:414:PRO:HD3	2.05	0.57
1:O:165:ASN:O	1:O:169:GLU:HG2	2.04	0.57
1:Q:112:THR:HG22	1:Q:113:GLU:OE2	2.05	0.57
3:T:84:DMF:C1	5:T:2221:HOH:O	2.52	0.57
1:B:155:VAL:HG12	1:B:160:THR:HG22	1.86	0.57
2:N:320:SER:HB3	2:N:331:VAL:HG21	1.87	0.57
2:E:509:ARG:CA	3:E:73:DMF:H12	2.34	0.57
1:M:155:VAL:HG12	1:M:160:THR:HG22	1.87	0.57
1:O:112:THR:HG22	1:O:113:GLU:OE2	2.05	0.57
1:S:155:VAL:HG12	1:S:160:THR:HG22	1.87	0.57
1:D:170:SER:CB	1:D:183:ILE:HG23	2.31	0.56
2:T:332:ARG:HB3	5:T:2540:HOH:O	2.05	0.56
1:A:170:SER:O	1:A:183:ILE:HD13	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:161:GLU:HB2	1:D:162:PRO:CD	2.30	0.56
2:J:412:SER:O	2:J:414:PRO:HD3	2.04	0.56
1:Q:163:ILE:HG23	1:Q:187:ALA:O	2.05	0.56
2:R:331:VAL:HG11	4:R:300:SA6:H19	1.87	0.56
1:Y:161:GLU:HB2	1:Y:162:PRO:CD	2.31	0.56
1:Y:205:VAL:HG23	1:Y:206:ALA:N	2.20	0.56
2:2:465:ARG:NH1	2:2:465:ARG:HG3	2.14	0.56
3:H:117:DMF:HC	5:H:555:HOH:O	2.06	0.56
1:W:92:ARG:HD3	1:W:129:HIS:CE1	2.40	0.56
2:2:509:ARG:NH1	3:2:52:DMF:O	2.29	0.56
1:D:178:THR:HG22	1:D:182:ARG:HE	1.71	0.56
1:F:9:PRO:HD2	1:M:15:GLU:HG2	1.88	0.56
1:I:7:ILE:HB	1:I:11:GLN:HB3	1.87	0.56
2:P:412:SER:O	2:P:414:PRO:HD3	2.05	0.56
1:1:189:ARG:NH1	1:1:203:LEU:N	2.53	0.56
1:O:178:THR:HG22	1:O:182:ARG:HE	1.70	0.56
1:Q:102:VAL:CG1	3:Q:249:DMF:H13	2.35	0.56
1:S:15:GLU:CB	1:1:9:PRO:HG2	2.36	0.56
1:Y:169:GLU:OE1	1:Y:169:GLU:HA	2.05	0.56
1:Q:76:ARG:HD3	5:Q:1459:HOH:O	2.03	0.56
1:F:102:VAL:HG12	3:F:250:DMF:H12	1.88	0.56
3:N:118:DMF:H22	3:V:32:DMF:HC	1.88	0.56
1:1:163:ILE:HG23	1:1:187:ALA:O	2.05	0.56
1:K:43:ALA:O	1:K:208:LEU:HD22	2.05	0.56
2:P:301:THR:N	4:P:300:SA6:HO6	2.02	0.56
3:G:24:DMF:H13	2:2:453:LEU:HD23	1.88	0.56
1:B:15:GLU:HG2	1:I:9:PRO:CD	2.32	0.56
2:L:412:SER:O	2:L:414:PRO:HD3	2.06	0.56
2:N:416:SER:HB2	5:V:2273:HOH:O	2.06	0.56
1:W:178:THR:HG22	1:W:182:ARG:HE	1.69	0.56
2:C:456:GLN:NE2	2:C:465:ARG:NH2	2.48	0.56
2:G:508:SER:O	2:G:512:GLU:HG3	2.06	0.56
1:M:7:ILE:O	1:M:9:PRO:HD3	2.07	0.56
2:T:452:LYS:HB3	3:T:102:DMF:H22	1.86	0.56
2:2:465:ARG:HH11	2:2:465:ARG:CG	2.12	0.55
2:G:412:SER:O	2:G:414:PRO:HD3	2.05	0.55
1:K:163:ILE:HG23	1:K:187:ALA:O	2.06	0.55
2:L:332:ARG:HD3	5:L:1905:HOH:O	2.06	0.55
1:1:178:THR:HG22	1:1:182:ARG:HE	1.70	0.55
1:A:8:SER:O	1:A:11:GLN:N	2.40	0.55
1:F:7:ILE:HG22	1:F:8:SER:N	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:15:GLU:HG3	1:Y:9:PRO:HG2	1.87	0.55
1:1:11:GLN:HA	1:1:11:GLN:NE2	2.22	0.55
1:I:19:LEU:HD11	1:S:13:MET:HG3	1.88	0.55
1:M:226:THR:HB	5:M:2302:HOH:O	2.07	0.55
1:U:231:GLN:O	1:U:234:LEU:HB2	2.05	0.55
1:1:226:THR:HG22	5:1:2558:HOH:O	2.07	0.55
1:Y:9:PRO:O	1:Y:12:ALA:HB3	2.06	0.55
1:D:163:ILE:HG23	1:D:187:ALA:O	2.07	0.55
2:N:412:SER:O	2:N:414:PRO:HD3	2.06	0.55
1:U:48:ARG:NE	5:U:2461:HOH:O	2.39	0.55
2:V:538:HIS:CD2	5:V:1790:HOH:O	2.54	0.55
2:J:433:GLU:HA	2:J:433:GLU:OE1	2.05	0.55
1:O:189:ARG:HG3	1:O:203:LEU:HD23	1.89	0.55
1:S:229:ALA:O	1:S:233:LEU:HD13	2.07	0.55
2:T:320:SER:HB3	2:T:331:VAL:HG21	1.87	0.55
3:C:103:DMF:H13	2:H:447:LYS:HZ1	1.70	0.55
1:Q:54:SER:CB	1:Q:75:ARG:HD2	2.37	0.55
2:V:320:SER:HB3	2:V:331:VAL:HG21	1.89	0.55
3:V:83:DMF:C1	5:V:1742:HOH:O	2.29	0.55
1:B:7:ILE:N	1:B:7:ILE:CD1	2.51	0.55
2:E:434:GLU:HG2	3:E:75:DMF:H23	1.89	0.55
2:V:430:ASN:ND2	3:V:82:DMF:C	2.70	0.55
1:A:54:SER:CB	1:A:75:ARG:HD2	2.37	0.55
1:M:161:GLU:HB2	1:M:162:PRO:CD	2.31	0.55
1:M:173:GLU:O	1:M:174:ASN:HB2	2.07	0.55
2:P:472:TYR:O	3:P:14:DMF:H13	2.07	0.55
1:F:7:ILE:CG2	1:F:11:GLN:CG	2.85	0.55
1:B:15:GLU:CG	1:I:9:PRO:CG	2.82	0.54
1:D:150:GLU:HG3	1:D:154:VAL:HG22	1.89	0.54
1:I:15:GLU:HG2	1:S:9:PRO:CG	2.37	0.54
1:B:174:ASN:HD22	1:B:174:ASN:N	2.04	0.54
2:E:461:ASP:OD2	2:E:509:ARG:NH2	2.37	0.54
1:S:142:THR:HG1	1:S:146:SER:HB2	1.70	0.54
2:V:444:LEU:HB2	5:V:1225:HOH:O	2.06	0.54
1:B:54:SER:CB	1:B:75:ARG:HD2	2.36	0.54
2:R:412:SER:O	2:R:414:PRO:HD3	2.06	0.54
1:S:163:ILE:HG23	1:S:187:ALA:O	2.06	0.54
1:I:161:GLU:HB2	1:I:162:PRO:CD	2.32	0.54
1:O:161:GLU:HB2	1:O:162:PRO:CD	2.31	0.54
1:A:80:GLN:HE21	1:A:81:PHE:N	2.00	0.54
1:B:150:GLU:HG3	1:B:154:VAL:HG22	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:111:PHE:CD1	1:M:143:TYR:HD1	2.25	0.54
1:Y:178:THR:HG22	1:Y:182:ARG:HE	1.72	0.54
1:F:178:THR:HG22	1:F:182:ARG:HE	1.71	0.54
1:F:97:ARG:CZ	5:F:2227:HOH:O	2.55	0.54
1:U:181:LEU:O	1:U:185:VAL:HG23	2.07	0.54
2:Z:412:SER:O	2:Z:414:PRO:HD3	2.07	0.54
1:O:152:HIS:HB3	1:O:171:TYR:CE2	2.43	0.54
3:T:102:DMF:H13	2:X:452:LYS:HB3	1.88	0.54
2:R:525:ASP:OD1	2:R:538:HIS:HE1	1.90	0.54
1:U:150:GLU:HG3	1:U:154:VAL:HG22	1.89	0.54
2:2:465:ARG:HG2	2:2:513:LEU:HD22	1.89	0.54
1:A:186:ALA:HA	1:A:189:ARG:HD3	1.89	0.54
2:E:333:LYS:HG2	4:E:300:SA6:H18	1.90	0.54
2:E:509:ARG:HA	3:E:73:DMF:H12	1.89	0.54
2:V:354:GLU:OE2	3:2:101:DMF:H13	2.08	0.54
2:E:320:SER:HB3	2:E:331:VAL:HG21	1.90	0.54
2:R:509:ARG:NH2	3:R:80:DMF:H11	2.23	0.54
1:Y:214:ASP:OD1	1:Y:214:ASP:C	2.46	0.54
1:M:19:LEU:HD23	1:M:19:LEU:O	2.08	0.53
2:N:417:ALA:HA	5:N:2031:HOH:O	2.08	0.53
3:U:250:DMF:N	3:V:27:DMF:H11	2.23	0.53
2:V:412:SER:O	2:V:414:PRO:HD3	2.07	0.53
1:W:170:SER:OG	1:W:183:ILE:HG23	2.08	0.53
2:2:433:GLU:OE1	3:2:108:DMF:H22	2.07	0.53
1:F:164:ALA:O	1:F:168:LYS:HG3	2.07	0.53
2:G:452:LYS:HD2	3:G:24:DMF:H11	1.90	0.53
2:G:445:PHE:H	3:G:64:DMF:C1	2.21	0.53
2:H:522:SER:HB2	5:L:2277:HOH:O	2.08	0.53
1:Q:13:MET:HG2	3:Q:250:DMF:H11	1.90	0.53
1:F:48:ARG:HH12	1:W:135:ARG:HB3	1.73	0.53
1:1:54:SER:CB	1:1:75:ARG:HD2	2.38	0.53
1:I:114:GLN:NE2	5:I:2530:HOH:O	2.30	0.53
1:Q:205:VAL:HG22	1:Q:230:LEU:HG	1.89	0.53
1:D:8:SER:HB2	1:Q:7:ILE:CG1	2.38	0.53
1:S:54:SER:CB	1:S:75:ARG:HD2	2.38	0.53
2:X:412:SER:O	2:X:414:PRO:HD3	2.09	0.53
1:B:141:ILE:N	1:B:141:ILE:HD12	2.23	0.53
2:G:445:PHE:CE2	3:G:64:DMF:H12	2.42	0.53
1:O:142:THR:OG1	1:O:146:SER:HB2	2.09	0.53
5:J:594:HOH:O	1:S:85:ARG:CG	2.56	0.53
1:U:155:VAL:HG12	1:U:160:THR:HG22	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:472:TYR:CZ	3:V:116:DMF:H13	2.43	0.53
1:Y:181:LEU:CD2	1:Y:233:LEU:HG	2.36	0.53
1:A:15:GLU:HG3	1:B:9:PRO:HD2	1.91	0.53
1:F:54:SER:CB	1:F:75:ARG:HD2	2.38	0.53
2:L:301:THR:N	4:L:300:SA6:HO6	2.07	0.53
2:V:496:ILE:HG21	3:V:39:DMF:H23	1.90	0.53
1:Y:17:SER:HG	1:Y:143:TYR:HH	1.53	0.53
1:A:150:GLU:HG3	1:A:154:VAL:HG22	1.91	0.53
1:B:74:LEU:HD12	3:B:249:DMF:H13	1.90	0.53
1:D:111:PHE:CE1	1:D:143:TYR:HD1	2.26	0.53
1:D:111:PHE:CE1	1:D:143:TYR:CD1	2.97	0.53
2:J:409:ILE:HG12	5:J:1416:HOH:O	2.09	0.53
2:R:386:MET:HE2	5:R:2543:HOH:O	2.08	0.53
2:V:380:ILE:HB	3:V:42:DMF:H23	1.90	0.53
1:W:155:VAL:HG12	1:W:160:THR:HG22	1.90	0.53
1:Y:91:ARG:HD2	3:Y:249:DMF:H11	1.91	0.53
1:B:174:ASN:ND2	1:B:174:ASN:N	2.54	0.53
1:B:181:LEU:HD23	1:B:233:LEU:HB2	1.91	0.53
1:K:155:VAL:HG12	1:K:160:THR:HG22	1.91	0.53
1:B:110:ILE:HG23	1:B:114:GLN:OE1	2.09	0.53
1:I:203:LEU:N	1:I:203:LEU:HD12	2.24	0.53
1:M:54:SER:CB	1:M:75:ARG:HD2	2.38	0.53
3:N:90:DMF:H21	3:V:120:DMF:HC	1.89	0.53
1:Y:150:GLU:HG3	1:Y:154:VAL:HG22	1.91	0.53
2:C:498:ASP:OD2	3:C:38:DMF:H12	2.08	0.53
1:I:150:GLU:HG3	1:I:154:VAL:HG22	1.90	0.53
1:W:141:ILE:HD12	1:W:141:ILE:N	2.23	0.53
1:A:112:THR:CG2	1:O:115:ALA:HB3	2.38	0.53
2:C:366:TYR:HD1	3:C:63:DMF:HC	1.74	0.53
2:P:515:ARG:NH2	5:P:1195:HOH:O	2.40	0.53
1:Q:219:ARG:NH2	3:Q:251:DMF:H22	2.23	0.53
1:S:150:GLU:HG3	1:S:154:VAL:HG22	1.91	0.53
1:D:16:ARG:NH1	1:D:117:PRO:HD3	2.25	0.52
1:D:137:GLU:HG2	1:Q:48:ARG:NH2	2.24	0.52
2:E:472:TYR:CD1	3:E:20:DMF:H12	2.43	0.52
1:M:179:ASP:O	1:M:183:ILE:HG13	2.09	0.52
1:M:231:GLN:HA	1:M:234:LEU:CD2	2.38	0.52
1:U:140:ARG:NH1	1:U:154:VAL:HG13	2.24	0.52
1:U:170:SER:OG	1:U:183:ILE:HG23	2.08	0.52
1:B:161:GLU:HB2	1:B:162:PRO:CD	2.32	0.52
2:T:412:SER:O	2:T:414:PRO:HD3	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:191:GLY:O	1:F:192:SER:HB2	2.09	0.52
1:F:7:ILE:CD1	1:W:8:SER:HB2	2.39	0.52
2:L:388:ARG:HD3	2:L:426:ALA:O	2.08	0.52
2:R:445:PHE:CE2	3:R:59:DMF:H12	2.45	0.52
1:O:9:PRO:CD	1:U:15:GLU:CG	2.64	0.52
1:Q:9:PRO:HD2	1:Y:15:GLU:HG3	1.91	0.52
1:1:155:VAL:HG12	1:1:160:THR:HG22	1.91	0.52
2:E:412:SER:O	2:E:414:PRO:HD3	2.09	0.52
1:F:225:ILE:HG21	1:F:233:LEU:HD12	1.91	0.52
1:K:54:SER:CB	1:K:75:ARG:HD2	2.39	0.52
1:M:189:ARG:O	1:M:190:ALA:C	2.47	0.52
1:Q:173:GLU:O	1:Q:174:ASN:HB2	2.08	0.52
1:W:150:GLU:HG3	1:W:154:VAL:HG22	1.91	0.52
1:Y:54:SER:CB	1:Y:75:ARG:HD2	2.39	0.52
1:F:155:VAL:HG12	1:F:160:THR:HG22	1.91	0.52
1:F:19:LEU:HD23	1:F:19:LEU:C	2.30	0.52
1:M:150:GLU:HG3	1:M:154:VAL:HG22	1.91	0.52
1:Q:90:ASP:HB3	1:Q:93:ASP:OD2	2.09	0.52
2:J:461:ASP:OD1	2:J:509:ARG:NH2	2.40	0.52
1:O:89:TYR:CD1	2:V:382:ARG:HD3	2.45	0.52
1:F:7:ILE:HG23	1:F:11:GLN:CD	2.30	0.52
1:M:152:HIS:HB3	1:M:171:TYR:CE2	2.45	0.52
1:U:54:SER:CB	1:U:75:ARG:HD2	2.40	0.52
1:1:8:SER:O	1:1:11:GLN:N	2.36	0.52
1:I:155:VAL:HG12	1:I:160:THR:HG22	1.91	0.52
1:K:15:GLU:OE2	1:M:10:GLU:HB3	2.10	0.52
1:O:54:SER:CB	1:O:75:ARG:HD2	2.39	0.52
1:D:13:MET:HE3	1:Q:19:LEU:HD11	1.92	0.52
1:B:170:SER:CB	1:B:183:ILE:HG23	2.40	0.52
2:J:465:ARG:HD2	3:J:123:DMF:H11	1.91	0.52
2:J:476:ASP:OD1	3:J:45:DMF:HC	2.10	0.52
1:K:114:GLN:OE1	3:K:252:DMF:H13	2.08	0.52
1:K:7:ILE:CG1	1:K:11:GLN:HE21	2.23	0.52
2:T:335:TYR:CB	3:T:29:DMF:H13	2.37	0.52
2:T:432:GLU:CD	2:T:437:GLN:HE21	2.14	0.52
1:1:182:ARG:NH1	1:1:234:LEU:O	2.42	0.51
1:A:87:TYR:CZ	2:H:358:LEU:HD13	2.45	0.51
2:V:434:GLU:HB2	3:V:32:DMF:H21	1.92	0.51
1:W:214:ASP:HB3	1:W:217:ARG:HG2	1.91	0.51
1:Y:135:ARG:HB2	1:Y:135:ARG:NH1	2.25	0.51
1:1:150:GLU:HG3	1:1:154:VAL:HG22	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:103:DMF:O	3:H:43:DMF:H22	2.10	0.51
1:D:179:ASP:O	1:D:183:ILE:HG13	2.10	0.51
1:S:141:ILE:N	1:S:141:ILE:HD12	2.25	0.51
1:W:87:TYR:CZ	2:X:358:LEU:HD13	2.45	0.51
1:B:8:SER:HB2	1:B:9:PRO:HD2	1.92	0.51
2:J:509:ARG:HG2	2:J:509:ARG:NH1	2.26	0.51
1:M:98:GLN:O	1:M:102:VAL:HG23	2.10	0.51
1:S:149:ASP:HB2	5:S:1142:HOH:O	2.11	0.51
1:W:97:ARG:NH2	5:W:1773:HOH:O	2.23	0.51
1:D:140:ARG:NH1	1:D:154:VAL:HG13	2.24	0.51
1:I:7:ILE:HB	1:I:11:GLN:CB	2.41	0.51
1:K:150:GLU:HG3	1:K:154:VAL:HG22	1.92	0.51
2:L:440:GLY:HA2	3:L:97:DMF:HC	1.92	0.51
2:T:349:ALA:HA	4:T:300:SA6:H17A	1.92	0.51
1:W:185:VAL:CG1	1:W:189:ARG:HH21	2.22	0.51
2:C:345:ILE:HB	2:C:352:ALA:HB1	1.91	0.51
1:D:144:ASP:OD2	1:D:146:SER:CB	2.59	0.51
1:F:187:ALA:O	1:F:190:ALA:HB3	2.11	0.51
2:J:465:ARG:HD2	3:J:123:DMF:C	2.39	0.51
1:K:44:GLU:HA	1:K:208:LEU:HD23	1.93	0.51
1:Q:155:VAL:HG12	1:Q:160:THR:HG22	1.91	0.51
1:Q:16:ARG:NE	3:Q:250:DMF:H22	2.24	0.51
1:S:8:SER:H	1:S:11:GLN:CB	2.21	0.51
3:V:116:DMF:HC	5:V:2127:HOH:O	2.08	0.51
1:A:181:LEU:O	1:A:185:VAL:HG23	2.11	0.51
1:F:150:GLU:HG3	1:F:154:VAL:HG22	1.93	0.51
1:Q:102:VAL:HG12	3:Q:249:DMF:H13	1.92	0.51
1:Y:77:GLY:HA3	3:Y:250:DMF:H23	1.93	0.51
1:A:56:LEU:HG	1:A:62:PHE:HB2	1.92	0.51
1:F:152:HIS:HB3	1:F:171:TYR:CE2	2.46	0.51
1:K:140:ARG:NH1	1:K:154:VAL:HG13	2.26	0.51
1:M:111:PHE:CE1	1:M:143:TYR:HE1	2.28	0.51
1:Q:87:TYR:O	2:R:357:ARG:NH1	2.42	0.51
1:Y:105:GLN:HB2	5:Y:1882:HOH:O	2.09	0.51
1:A:182:ARG:HH11	1:A:234:LEU:HA	1.74	0.51
1:I:8:SER:O	1:I:12:ALA:N	2.39	0.51
1:S:189:ARG:O	1:S:190:ALA:C	2.48	0.51
1:D:155:VAL:HG12	1:D:160:THR:HG22	1.92	0.51
1:S:179:ASP:O	1:S:183:ILE:HG13	2.11	0.51
2:V:332:ARG:HD3	5:V:2665:HOH:O	2.11	0.51
5:O:2444:HOH:O	3:V:42:DMF:C	2.59	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:511:ALA:O	2:C:515:ARG:HG3	2.11	0.51
2:E:392:ALA:HA	2:E:395:MET:HE2	1.93	0.51
1:I:140:ARG:NH1	1:I:154:VAL:HG13	2.26	0.51
2:J:332:ARG:HD3	5:J:545:HOH:O	2.10	0.51
2:L:432:GLU:HG2	2:L:437:GLN:HB2	1.93	0.51
3:P:2:DMF:C	5:P:791:HOH:O	2.59	0.51
1:U:9:PRO:HD2	1:I:15:GLU:CG	2.40	0.51
1:Y:155:VAL:HG12	1:Y:160:THR:HG22	1.93	0.51
1:B:233:LEU:CD1	1:B:233:LEU:N	2.63	0.50
1:F:165:ASN:O	1:F:169:GLU:HG2	2.11	0.50
2:G:447:LYS:HD3	3:G:119:DMF:H23	1.87	0.50
1:K:135:ARG:NH1	1:K:135:ARG:HB2	2.26	0.50
1:U:167:LEU:HG	1:U:187:ALA:CB	2.42	0.50
1:I:54:SER:CB	1:I:75:ARG:HD2	2.41	0.50
2:J:515:ARG:NH1	2:R:539:HIS:N	2.54	0.50
1:O:155:VAL:HG12	1:O:160:THR:HG22	1.93	0.50
1:Q:174:ASN:N	1:Q:174:ASN:HD22	2.10	0.50
1:S:140:ARG:NH1	1:S:154:VAL:HG13	2.25	0.50
1:W:135:ARG:NH1	1:W:135:ARG:HB2	2.27	0.50
1:Q:13:MET:CG	1:Y:19:LEU:HD11	2.39	0.50
2:2:465:ARG:NH1	2:2:465:ARG:CG	2.74	0.50
1:A:163:ILE:HG23	1:A:187:ALA:O	2.11	0.50
1:A:54:SER:HB2	5:A:2123:HOH:O	2.11	0.50
1:M:166:ALA:O	1:M:170:SER:OG	2.25	0.50
2:V:525:ASP:OD2	2:V:538:HIS:HE1	1.94	0.50
1:W:179:ASP:O	1:W:183:ILE:HG13	2.10	0.50
1:I:56:LEU:HG	1:I:62:PHE:HB2	1.93	0.50
3:V:83:DMF:H11	3:2:4:DMF:HC	1.92	0.50
1:O:172:ALA:O	1:O:175:ALA:HB2	2.12	0.50
1:W:116:LYS:NZ	1:W:117:PRO:O	2.45	0.50
1:B:140:ARG:NH1	1:B:154:VAL:HG13	2.26	0.50
1:D:108:GLY:C	3:D:251:DMF:C2	2.80	0.50
2:X:336:ILE:O	3:X:16:DMF:H13	2.11	0.50
1:Y:179:ASP:O	1:Y:183:ILE:HG13	2.11	0.50
1:D:144:ASP:OD2	1:D:146:SER:OG	2.30	0.50
1:D:173:GLU:C	1:D:174:ASN:ND2	2.63	0.50
2:V:477:ASP:OD2	5:V:2199:HOH:O	2.20	0.50
1:F:48:ARG:NH2	1:W:136:PRO:O	2.45	0.50
1:W:11:GLN:HG2	1:W:14:ARG:NH2	2.27	0.50
1:K:161:GLU:HB2	1:K:162:PRO:CD	2.31	0.50
1:M:135:ARG:NH1	1:M:135:ARG:HB2	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:56:LEU:HG	1:Y:62:PHE:HB2	1.93	0.50
2:C:509:ARG:HG2	5:C:2378:HOH:O	2.10	0.49
2:H:333:LYS:HG2	4:H:300:SA6:H18	1.94	0.49
1:I:141:ILE:HD12	1:I:141:ILE:N	2.27	0.49
1:K:102:VAL:HG22	3:K:251:DMF:HC	1.92	0.49
1:Q:7:ILE:CG2	1:Q:8:SER:H	2.24	0.49
1:D:54:SER:CB	1:D:75:ARG:HD2	2.42	0.49
1:F:165:ASN:HA	1:F:168:LYS:HD2	1.95	0.49
1:F:173:GLU:O	1:F:174:ASN:HB2	2.11	0.49
2:H:324:ASN:HB2	5:H:2206:HOH:O	2.11	0.49
1:O:52:LYS:NZ	5:O:2621:HOH:O	2.45	0.49
1:Y:10:GLU:O	1:Y:10:GLU:OE1	2.30	0.49
1:Y:140:ARG:NH1	1:Y:154:VAL:HG13	2.27	0.49
1:I:225:ILE:HG21	1:I:233:LEU:HD12	1.94	0.49
1:A:140:ARG:NH1	1:A:154:VAL:HG13	2.27	0.49
1:A:155:VAL:HG12	1:A:160:THR:HG22	1.94	0.49
1:B:16:ARG:NH2	1:B:114:GLN:O	2.29	0.49
2:G:430:ASN:HD22	3:G:98:DMF:C	2.23	0.49
1:I:233:LEU:HD12	1:I:233:LEU:N	2.27	0.49
1:U:33:LEU:HD12	1:U:33:LEU:O	2.13	0.49
1:W:144:ASP:OD1	1:W:146:SER:OG	2.30	0.49
1:W:91:ARG:NH1	3:W:250:DMF:HC	2.27	0.49
2:C:413:ASP:HB3	5:C:2547:HOH:O	2.12	0.49
3:V:83:DMF:H23	5:V:2660:HOH:O	2.11	0.49
1:D:135:ARG:NH1	1:D:135:ARG:HB2	2.27	0.49
1:W:142:THR:OG1	1:W:144:ASP:OD2	2.30	0.49
1:W:140:ARG:NH1	1:W:154:VAL:HG13	2.28	0.49
1:A:163:ILE:HG22	1:A:187:ALA:HB1	1.93	0.49
1:M:183:ILE:HD11	5:M:2226:HOH:O	2.12	0.49
2:G:445:PHE:H	3:G:64:DMF:H13	1.77	0.49
1:M:56:LEU:HG	1:M:62:PHE:HB2	1.95	0.49
1:Q:150:GLU:HG3	1:Q:154:VAL:HG22	1.93	0.49
1:U:144:ASP:OD1	1:U:146:SER:OG	2.30	0.49
3:V:116:DMF:C	5:V:1032:HOH:O	2.60	0.49
1:Y:85:ARG:NH2	5:Y:1296:HOH:O	2.39	0.49
2:2:412:SER:O	2:2:414:PRO:HD3	2.13	0.49
1:D:204:GLY:O	1:D:208:LEU:HG	2.12	0.49
2:E:465:ARG:NH2	5:E:2061:HOH:O	2.45	0.49
1:F:185:VAL:O	1:F:189:ARG:HB2	2.11	0.49
2:L:374:LEU:HD21	1:M:89:TYR:CD1	2.48	0.49
1:Q:16:ARG:CD	3:Q:250:DMF:H22	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:443:SER:N	3:R:59:DMF:HC	2.28	0.49
2:H:392:ALA:N	5:H:2626:HOH:O	2.36	0.49
1:I:56:LEU:HG	1:I:62:PHE:HB2	1.94	0.49
2:P:333:LYS:HG2	4:P:300:SA6:H18	1.95	0.49
2:R:456:GLN:NE2	2:R:465:ARG:NH2	2.56	0.49
1:Y:167:LEU:HG	1:Y:187:ALA:CB	2.43	0.49
2:2:432:GLU:OE2	2:2:434:GLU:HB2	2.13	0.49
1:D:142:THR:OG1	1:D:144:ASP:OD2	2.30	0.49
1:S:56:LEU:HG	1:S:62:PHE:HB2	1.95	0.49
1:Y:181:LEU:HD22	1:Y:233:LEU:CD2	2.42	0.49
1:1:19:LEU:HD23	1:1:19:LEU:C	2.32	0.48
1:K:167:LEU:HG	1:K:187:ALA:CB	2.43	0.48
1:Q:135:ARG:NH1	1:Q:135:ARG:HB2	2.28	0.48
1:S:14:ARG:HH21	1:S:14:ARG:HG2	1.79	0.48
1:Y:142:THR:OG1	1:Y:144:ASP:OD1	2.30	0.48
3:T:113:DMF:C1	3:2:112:DMF:C	2.86	0.48
1:B:15:GLU:CG	1:I:9:PRO:CD	2.90	0.48
1:B:56:LEU:HG	1:B:62:PHE:HB2	1.94	0.48
1:D:144:ASP:OD1	1:D:146:SER:OG	2.30	0.48
1:I:179:ASP:O	1:I:183:ILE:HG13	2.13	0.48
2:L:472:TYR:CZ	3:L:81:DMF:H11	2.48	0.48
1:Q:33:LEU:HD12	1:Q:33:LEU:O	2.13	0.48
3:V:83:DMF:C2	2:2:447:LYS:HZ2	2.24	0.48
1:Y:110:ILE:HG23	1:Y:114:GLN:NE2	2.28	0.48
1:1:140:ARG:NH1	1:1:154:VAL:HG13	2.28	0.48
2:E:444:LEU:HD21	2:L:325:MET:SD	2.54	0.48
1:M:140:ARG:NH1	1:M:154:VAL:HG13	2.28	0.48
2:N:382:ARG:NH2	2:N:385:ILE:CD1	2.77	0.48
1:O:150:GLU:HG3	1:O:154:VAL:HG22	1.95	0.48
1:Q:167:LEU:HG	1:Q:187:ALA:CB	2.43	0.48
1:S:15:GLU:OE1	1:1:8:SER:CB	2.60	0.48
2:X:429:TRP:CH2	3:X:41:DMF:H12	2.47	0.48
2:Z:331:VAL:HG11	4:Z:300:SA6:H19	1.95	0.48
2:2:345:ILE:HB	2:2:352:ALA:HB1	1.95	0.48
2:E:436:TYR:CZ	3:E:75:DMF:H22	2.47	0.48
2:N:515:ARG:O	2:N:519:GLU:HG3	2.14	0.48
1:Q:140:ARG:NH1	1:Q:154:VAL:HG13	2.28	0.48
2:J:515:ARG:HH12	2:R:539:HIS:H	1.56	0.48
3:Z:18:DMF:H13	5:Z:932:HOH:O	2.12	0.48
1:B:142:THR:OG1	1:B:146:SER:HB2	2.13	0.48
2:C:416:SER:HB2	2:R:533:GLU:HB2	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:170:SER:HB2	1:D:183:ILE:CG2	2.35	0.48
2:G:444:LEU:H	3:G:64:DMF:C	2.27	0.48
1:M:111:PHE:CE1	1:M:143:TYR:HD1	2.30	0.48
1:M:152:HIS:HB3	1:M:171:TYR:CZ	2.48	0.48
2:N:483:GLY:HA3	3:N:22:DMF:H22	1.95	0.48
3:V:83:DMF:H22	2:2:447:LYS:CE	2.42	0.48
1:F:7:ILE:HG23	1:F:11:GLN:OE1	2.12	0.48
1:U:152:HIS:HB3	1:U:171:TYR:CE2	2.48	0.48
3:T:102:DMF:H11	2:X:452:LYS:O	2.13	0.48
2:2:333:LYS:HG2	4:2:300:SA6:H18	1.94	0.48
3:C:38:DMF:H21	5:C:1447:HOH:O	2.13	0.48
1:F:81:PHE:CZ	1:F:102:VAL:HG21	2.49	0.48
1:F:52:LYS:NZ	5:F:2647:HOH:O	2.46	0.48
1:K:15:GLU:CG	1:M:9:PRO:HD2	2.31	0.48
2:R:325:MET:CE	2:Z:444:LEU:HD11	2.44	0.48
1:1:19:LEU:O	1:1:19:LEU:HD23	2.13	0.48
1:S:15:GLU:OE2	1:1:8:SER:HB3	2.13	0.48
1:F:161:GLU:HB2	1:F:162:PRO:CD	2.32	0.48
1:F:97:ARG:NH2	5:F:2383:HOH:O	2.46	0.48
1:S:149:ASP:HB3	5:S:1142:HOH:O	2.13	0.48
1:1:167:LEU:HG	1:1:187:ALA:CB	2.43	0.48
1:O:90:ASP:HB3	1:O:93:ASP:OD2	2.13	0.48
1:S:19:LEU:C	1:S:19:LEU:HD23	2.35	0.48
1:U:229:ALA:O	1:U:233:LEU:HD13	2.14	0.48
1:1:135:ARG:HB2	1:1:135:ARG:NH1	2.29	0.48
1:B:135:ARG:HB2	1:B:135:ARG:NH1	2.29	0.48
1:D:56:LEU:HG	1:D:62:PHE:HB2	1.95	0.48
1:F:135:ARG:NH1	1:F:135:ARG:HB2	2.29	0.48
1:S:205:VAL:HG22	1:S:205:VAL:O	2.13	0.48
2:T:382:ARG:NH2	2:T:385:ILE:HD13	2.28	0.48
1:I:52:LYS:NZ	5:I:2616:HOH:O	2.46	0.47
1:M:144:ASP:OD1	1:M:146:SER:OG	2.30	0.47
1:M:11:GLN:HG2	1:M:14:ARG:HH22	1.79	0.47
2:P:508:SER:O	2:P:512:GLU:HG3	2.14	0.47
1:Q:233:LEU:N	1:Q:233:LEU:HD22	2.29	0.47
1:A:135:ARG:NH1	1:A:135:ARG:HB2	2.29	0.47
1:Q:13:MET:HG3	1:Y:19:LEU:CD1	2.38	0.47
2:V:306:LEU:HD12	2:V:306:LEU:C	2.34	0.47
1:Y:228:SER:O	1:Y:231:GLN:HB3	2.14	0.47
1:A:170:SER:OG	1:A:183:ILE:HG23	2.14	0.47
2:H:392:ALA:HB3	5:H:7:HOH:O	2.12	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:52:LYS:NZ	5:M:437:HOH:O	2.46	0.47
1:O:135:ARG:NH1	1:O:135:ARG:HB2	2.29	0.47
2:R:445:PHE:H	3:R:59:DMF:C1	2.27	0.47
1:S:33:LEU:HD12	1:S:33:LEU:O	2.14	0.47
1:1:161:GLU:HB2	1:1:162:PRO:CD	2.31	0.47
1:A:163:ILE:HG23	1:A:187:ALA:CB	2.43	0.47
2:G:437:GLN:NE2	3:G:119:DMF:H12	2.29	0.47
1:K:179:ASP:O	1:K:183:ILE:HG13	2.15	0.47
2:P:351:VAL:HG21	2:P:398:LEU:HB3	1.95	0.47
2:V:398:LEU:CD1	2:V:398:LEU:N	2.78	0.47
1:1:166:ALA:O	1:1:170:SER:OG	2.22	0.47
2:X:477:ASP:HB3	3:2:112:DMF:H11	1.97	0.47
1:A:226:THR:HG22	5:A:1272:HOH:O	2.15	0.47
1:B:7:ILE:HG23	1:B:11:GLN:HG2	1.88	0.47
1:I:228:SER:O	1:I:231:GLN:HB3	2.15	0.47
1:F:56:LEU:HG	1:F:62:PHE:HB2	1.96	0.47
1:F:7:ILE:CG2	1:F:11:GLN:CD	2.83	0.47
1:B:15:GLU:HG2	1:I:9:PRO:HG2	1.94	0.47
1:O:33:LEU:HD12	1:O:33:LEU:O	2.14	0.47
1:S:144:ASP:OD1	1:S:146:SER:OG	2.30	0.47
2:X:333:LYS:HG2	4:X:300:SA6:H18	1.95	0.47
1:O:140:ARG:NH1	1:O:154:VAL:HG13	2.29	0.47
2:2:484:PRO:HD2	5:2:2503:HOH:O	2.15	0.47
1:B:179:ASP:O	1:B:183:ILE:HG13	2.14	0.47
2:C:372:VAL:HG23	2:C:373:PRO:HD2	1.97	0.47
1:F:7:ILE:HG21	1:F:11:GLN:HG2	1.97	0.47
1:I:135:ARG:NH1	1:I:135:ARG:HB2	2.30	0.47
1:U:135:ARG:NH1	1:U:135:ARG:HB2	2.29	0.47
4:V:300:SA6:H1B	4:V:300:SA6:O6	2.15	0.47
2:2:388:ARG:NH1	5:2:2358:HOH:O	2.46	0.47
2:X:306:LEU:C	2:X:306:LEU:HD12	2.34	0.47
1:O:179:ASP:O	1:O:183:ILE:HG13	2.15	0.47
1:S:102:VAL:HG12	3:S:249:DMF:H12	1.97	0.47
1:S:52:LYS:HE2	1:S:64:ALA:O	2.15	0.47
1:S:80:GLN:NE2	5:S:2220:HOH:O	2.48	0.47
1:F:15:GLU:HG2	1:W:9:PRO:HG2	1.96	0.47
1:D:8:SER:HG	1:D:9:PRO:HD3	1.80	0.47
1:S:169:GLU:OE1	1:S:169:GLU:CA	2.62	0.47
1:S:228:SER:O	1:S:231:GLN:HB3	2.15	0.47
2:C:498:ASP:OD2	3:C:38:DMF:C1	2.63	0.46
1:D:167:LEU:HG	1:D:187:ALA:CB	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:33:LEU:HD12	1:K:33:LEU:O	2.14	0.46
1:S:135:ARG:NH1	1:S:135:ARG:HB2	2.30	0.46
1:U:231:GLN:HA	1:U:234:LEU:HD12	1.97	0.46
2:X:331:VAL:HG11	4:X:300:SA6:C19	2.43	0.46
2:C:333:LYS:HG2	4:C:300:SA6:H18	1.97	0.46
2:G:432:GLU:OE1	3:G:119:DMF:H11	2.14	0.46
1:K:228:SER:O	1:K:231:GLN:HB3	2.15	0.46
1:Q:20:ALA:O	1:Q:24:ILE:HG13	2.15	0.46
2:C:416:SER:CB	2:R:533:GLU:HB2	2.45	0.46
1:U:161:GLU:HB2	1:U:162:PRO:CD	2.31	0.46
2:G:306:LEU:HD12	2:G:306:LEU:C	2.36	0.46
1:O:19:LEU:HD23	1:O:19:LEU:O	2.16	0.46
1:U:8:SER:HA	1:U:9:PRO:HD2	1.71	0.46
2:V:377:ALA:O	3:V:42:DMF:H23	2.16	0.46
1:Y:13:MET:HE3	1:Y:13:MET:HA	1.97	0.46
2:C:301:THR:HG22	2:C:302:THR:N	2.30	0.46
1:F:33:LEU:HD12	1:F:33:LEU:O	2.15	0.46
1:I:167:LEU:HG	1:I:187:ALA:CB	2.45	0.46
2:J:382:ARG:NH2	2:J:385:ILE:CD1	2.79	0.46
2:L:320:SER:HB3	2:L:331:VAL:HG21	1.96	0.46
1:Q:142:THR:HA	5:Q:2537:HOH:O	2.16	0.46
1:D:109:THR:N	3:D:251:DMF:C2	2.75	0.46
2:N:333:LYS:HG2	4:N:300:SA6:H18	1.98	0.46
1:O:189:ARG:CG	1:O:203:LEU:HD23	2.41	0.46
2:R:306:LEU:C	2:R:306:LEU:HD12	2.36	0.46
1:S:11:GLN:OE1	1:S:14:ARG:HD3	2.15	0.46
1:S:178:THR:CG2	1:S:182:ARG:HE	2.28	0.46
2:V:483:GLY:HA3	3:V:116:DMF:C2	2.43	0.46
1:W:26:ARG:CG	1:W:26:ARG:O	2.64	0.46
1:W:90:ASP:HB3	1:W:93:ASP:OD2	2.15	0.46
3:X:15:DMF:C1	5:X:1898:HOH:O	2.63	0.46
1:Y:110:ILE:HG23	1:Y:114:GLN:HE21	1.80	0.46
1:D:16:ARG:NH2	1:D:114:GLN:O	2.40	0.46
3:G:12:DMF:C1	5:V:723:HOH:O	2.63	0.46
1:I:170:SER:O	1:I:183:ILE:HD13	2.16	0.46
2:J:382:ARG:NH2	2:J:385:ILE:HD13	2.31	0.46
2:J:415:GLN:NE2	5:J:1604:HOH:O	2.47	0.46
1:D:15:GLU:HG2	1:K:9:PRO:HD2	1.97	0.46
1:O:133:THR:HA	5:O:1191:HOH:O	2.15	0.46
1:A:9:PRO:CD	1:O:15:GLU:HG2	2.46	0.46
2:R:477:ASP:OD2	5:R:2581:HOH:O	2.20	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:56:LEU:HG	1:W:62:PHE:HB2	1.98	0.46
1:1:179:ASP:O	1:1:183:ILE:HG13	2.16	0.46
1:A:167:LEU:HD23	1:A:167:LEU:HA	1.82	0.46
2:H:432:GLU:OE2	2:H:434:GLU:HG3	2.16	0.46
2:J:516:ALA:O	3:J:123:DMF:H23	2.14	0.46
2:L:309:PRO:HB2	5:L:1576:HOH:O	2.14	0.46
1:1:8:SER:O	1:1:11:GLN:HB3	2.15	0.46
2:G:521:ARG:HB3	3:G:70:DMF:H11	1.97	0.46
1:M:142:THR:OG1	1:M:144:ASP:OD2	2.30	0.46
2:R:325:MET:HE2	2:R:325:MET:HB3	1.63	0.46
2:T:360:ALA:CB	3:T:29:DMF:H23	2.46	0.46
1:U:56:LEU:HG	1:U:62:PHE:HB2	1.98	0.46
1:D:109:THR:OG1	3:D:251:DMF:H13	2.15	0.46
1:D:111:PHE:CD1	1:D:143:TYR:HD1	2.34	0.46
1:D:33:LEU:HD12	1:D:33:LEU:O	2.16	0.46
1:I:233:LEU:HD11	5:I:1562:HOH:O	2.16	0.46
3:N:90:DMF:C2	3:V:120:DMF:H12	2.43	0.46
1:I:19:LEU:HD21	1:S:13:MET:HE1	1.98	0.46
2:X:409:ILE:HG12	5:X:2539:HOH:O	2.15	0.46
2:Z:391:LEU:O	2:Z:395:MET:HG3	2.15	0.46
1:B:226:THR:HG22	5:B:1667:HOH:O	2.16	0.46
1:K:178:THR:CG2	1:K:182:ARG:HE	2.28	0.46
1:W:185:VAL:HG12	1:W:189:ARG:HH21	1.79	0.46
1:Y:178:THR:CG2	1:Y:182:ARG:HE	2.29	0.46
1:Y:170:SER:OG	1:Y:183:ILE:HG23	2.15	0.46
1:Y:33:LEU:HD12	1:Y:33:LEU:O	2.16	0.46
1:A:230:LEU:O	1:A:234:LEU:CD2	2.60	0.45
1:B:178:THR:CG2	1:B:182:ARG:HE	2.29	0.45
1:B:19:LEU:HD23	1:B:19:LEU:C	2.36	0.45
1:D:76:ARG:HD3	5:D:546:HOH:O	2.16	0.45
1:I:162:PRO:HB3	1:I:190:ALA:O	2.16	0.45
1:O:203:LEU:N	1:O:203:LEU:HD22	2.31	0.45
2:C:444:LEU:HD21	2:J:325:MET:SD	2.56	0.45
1:D:107:LEU:HD12	1:D:141:ILE:CG2	2.47	0.45
1:I:170:SER:HB2	1:I:183:ILE:HG23	1.99	0.45
1:O:189:ARG:O	1:O:190:ALA:C	2.55	0.45
2:Z:333:LYS:HG2	4:Z:300:SA6:H18	1.98	0.45
1:1:228:SER:O	1:1:231:GLN:HB3	2.16	0.45
1:D:116:LYS:NZ	1:D:119:GLU:OE2	2.47	0.45
1:F:19:LEU:O	1:F:19:LEU:HD23	2.16	0.45
3:2:108:DMF:C1	5:2:1666:HOH:O	2.65	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:307:LYS:HE3	2:C:418:GLY:O	2.16	0.45
2:G:333:LYS:HG2	4:G:300:SA6:H18	1.98	0.45
1:M:52:LYS:HE2	1:M:64:ALA:O	2.17	0.45
1:W:52:LYS:HE2	1:W:64:ALA:O	2.17	0.45
1:F:179:ASP:O	1:F:183:ILE:HG13	2.17	0.45
2:L:333:LYS:HG2	4:L:300:SA6:H18	1.98	0.45
2:L:456:GLN:NE2	2:L:465:ARG:HH22	2.14	0.45
1:M:178:THR:CG2	1:M:182:ARG:HE	2.30	0.45
1:D:9:PRO:HD2	1:Q:15:GLU:HG3	1.98	0.45
3:T:84:DMF:H13	5:T:2221:HOH:O	2.15	0.45
1:W:16:ARG:NH1	1:W:117:PRO:HD3	2.31	0.45
1:Y:121:GLU:CG	5:Y:2504:HOH:O	2.58	0.45
1:M:33:LEU:O	1:M:33:LEU:HD12	2.16	0.45
1:S:19:LEU:HD23	1:S:19:LEU:O	2.17	0.45
1:I:102:VAL:CG1	3:I:250:DMF:H12	2.41	0.45
1:M:110:ILE:HA	1:M:114:GLN:HG3	1.98	0.45
2:N:399:LEU:HD12	2:N:400:ALA:N	2.32	0.45
1:O:56:LEU:HG	1:O:62:PHE:HB2	1.98	0.45
1:O:76:ARG:NH1	5:O:1434:HOH:O	2.35	0.45
1:W:81:PHE:CZ	1:W:102:VAL:HG21	2.52	0.45
1:W:77:GLY:HA3	3:W:249:DMF:C1	2.44	0.45
1:Y:169:GLU:OE1	1:Y:169:GLU:CA	2.63	0.45
1:I:178:THR:CG2	1:I:182:ARG:HE	2.30	0.45
1:F:141:ILE:N	1:F:141:ILE:HD12	2.32	0.45
1:I:178:THR:CG2	1:I:182:ARG:NH2	2.80	0.45
1:M:17:SER:OG	1:M:143:TYR:OH	2.23	0.45
1:M:228:SER:O	1:M:231:GLN:HB3	2.16	0.45
1:Q:13:MET:SD	3:Q:250:DMF:H12	2.54	0.45
1:Q:8:SER:O	1:Q:11:GLN:N	2.48	0.45
1:U:144:ASP:CG	1:U:146:SER:HG	2.19	0.45
2:X:362:GLU:OE2	2:X:382:ARG:NE	2.49	0.45
1:F:85:ARG:NH2	5:F:1784:HOH:O	2.49	0.45
2:N:372:VAL:HG23	2:N:373:PRO:HD2	1.99	0.45
1:O:178:THR:CG2	1:O:182:ARG:HE	2.30	0.45
2:R:534:LYS:NZ	3:R:92:DMF:O	2.50	0.45
1:W:72:ASP:O	1:W:76:ARG:HG3	2.17	0.45
2:C:307:LYS:HD3	2:R:530:ASP:OD1	2.17	0.44
2:N:456:GLN:NE2	2:N:465:ARG:NH2	2.51	0.44
1:I:45:ASN:HA	1:I:46:PRO:HD2	1.90	0.44
1:A:8:SER:O	1:A:11:GLN:HB3	2.18	0.44
1:F:228:SER:O	1:F:231:GLN:HB3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:151:PRO:HD2	5:K:1959:HOH:O	2.17	0.44
1:K:44:GLU:HA	1:K:208:LEU:CD2	2.47	0.44
2:L:396:GLN:HA	2:L:396:GLN:OE1	2.16	0.44
1:S:111:PHE:CE1	1:S:143:TYR:CE1	3.05	0.44
1:B:74:LEU:HA	3:B:249:DMF:H12	1.99	0.44
2:C:432:GLU:HB3	5:C:1566:HOH:O	2.16	0.44
2:E:301:THR:HG22	2:E:302:THR:N	2.32	0.44
2:T:392:ALA:HB3	5:T:1471:HOH:O	2.17	0.44
1:U:85:ARG:NH2	5:U:2357:HOH:O	2.50	0.44
2:X:392:ALA:HB3	5:X:1744:HOH:O	2.16	0.44
1:D:13:MET:CE	1:Q:19:LEU:HD11	2.48	0.44
2:R:444:LEU:H	3:R:59:DMF:HC	1.82	0.44
1:S:234:LEU:O	1:S:235:VAL:HG13	2.17	0.44
2:V:392:ALA:HA	2:V:395:MET:CE	2.48	0.44
2:V:392:ALA:HA	2:V:395:MET:HE2	2.00	0.44
1:B:24:ILE:HD11	1:B:120:VAL:O	2.17	0.44
1:D:166:ALA:O	1:D:170:SER:OG	2.32	0.44
1:D:52:LYS:HE2	1:D:64:ALA:O	2.18	0.44
2:E:374:LEU:HD21	1:K:89:TYR:CD1	2.52	0.44
1:M:213:LEU:HD23	1:M:213:LEU:HA	1.89	0.44
2:N:381:ASN:HB2	3:N:93:DMF:H21	1.99	0.44
1:S:167:LEU:HG	1:S:187:ALA:HB1	1.98	0.44
1:U:167:LEU:HG	1:U:187:ALA:HB1	1.99	0.44
1:W:114:GLN:O	1:W:115:ALA:C	2.56	0.44
2:X:372:VAL:HG23	2:X:373:PRO:HD2	1.99	0.44
1:I:81:PHE:CZ	1:I:102:VAL:HG21	2.53	0.44
2:2:419:ARG:NH1	3:2:108:DMF:HC	2.33	0.44
1:A:186:ALA:HA	1:A:189:ARG:CD	2.47	0.44
2:H:306:LEU:HD12	2:H:306:LEU:C	2.38	0.44
1:O:52:LYS:HE2	1:O:64:ALA:O	2.17	0.44
2:V:325:MET:SD	2:2:444:LEU:HD21	2.57	0.44
2:E:392:ALA:HA	2:E:395:MET:CE	2.48	0.44
2:E:433:GLU:HG3	2:L:330:ASP:CG	2.39	0.44
1:I:56:LEU:HA	1:I:56:LEU:HD23	1.85	0.44
1:I:8:SER:H	1:I:11:GLN:HB2	1.83	0.44
2:J:444:LEU:HB3	5:J:764:HOH:O	2.17	0.44
2:2:434:GLU:HB3	3:2:4:DMF:H23	1.94	0.44
1:D:228:SER:O	1:D:231:GLN:HB3	2.17	0.44
1:I:16:ARG:NH2	1:I:114:GLN:O	2.37	0.44
2:R:351:VAL:HG21	2:R:398:LEU:O	2.18	0.44
1:Y:19:LEU:HD23	1:Y:19:LEU:C	2.37	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:306:LEU:HD12	2:C:306:LEU:C	2.37	0.43
1:D:189:ARG:CG	5:D:2659:HOH:O	2.65	0.43
1:F:203:LEU:HA	1:F:203:LEU:HD23	1.89	0.43
1:F:7:ILE:CG2	1:F:8:SER:N	2.81	0.43
2:G:432:GLU:CD	3:G:119:DMF:H11	2.37	0.43
2:G:443:SER:N	3:G:64:DMF:HC	2.32	0.43
2:J:372:VAL:HG23	2:J:373:PRO:HD2	1.99	0.43
1:M:48:ARG:NH2	5:M:2620:HOH:O	2.44	0.43
2:N:416:SER:CB	2:V:533:GLU:HB2	2.48	0.43
1:O:170:SER:OG	1:O:183:ILE:HG23	2.18	0.43
1:D:99:LEU:HA	1:D:99:LEU:HD13	1.91	0.43
1:K:7:ILE:HG23	1:K:8:SER:N	2.32	0.43
2:L:507:GLU:OE2	5:L:72:HOH:O	2.21	0.43
2:N:429:TRP:CE2	3:N:93:DMF:HC	2.49	0.43
1:Q:19:LEU:C	1:Q:19:LEU:HD23	2.38	0.43
1:Q:52:LYS:HE2	1:Q:64:ALA:O	2.18	0.43
1:A:213:LEU:HD23	1:A:213:LEU:HA	1.88	0.43
1:B:213:LEU:HA	1:B:213:LEU:HD23	1.88	0.43
1:F:205:VAL:HG22	1:F:230:LEU:HG	1.99	0.43
2:G:472:TYR:CZ	3:G:12:DMF:H22	2.53	0.43
1:I:26:ARG:CG	1:I:26:ARG:O	2.65	0.43
2:J:396:GLN:CA	2:J:396:GLN:OE1	2.61	0.43
2:R:442:GLY:C	3:R:59:DMF:H11	2.39	0.43
1:S:116:LYS:HG2	1:S:117:PRO:O	2.18	0.43
1:B:110:ILE:HG12	1:B:114:GLN:OE1	2.18	0.43
2:E:345:ILE:HD12	2:E:352:ALA:O	2.18	0.43
2:V:380:ILE:HG22	3:V:42:DMF:H22	1.99	0.43
1:W:7:ILE:HG12	1:W:8:SER:N	2.31	0.43
2:2:372:VAL:HG23	2:2:373:PRO:HD2	2.01	0.43
1:A:228:SER:O	1:A:231:GLN:HB3	2.18	0.43
1:F:52:LYS:HE2	1:F:64:ALA:O	2.18	0.43
1:I:33:LEU:O	1:I:33:LEU:HD12	2.19	0.43
2:N:435:GLY:HA2	2:V:530:ASP:OD1	2.19	0.43
1:O:45:ASN:HA	1:O:46:PRO:HD2	1.88	0.43
1:Q:13:MET:SD	3:Q:250:DMF:H11	2.57	0.43
1:Q:228:SER:O	1:Q:231:GLN:HB3	2.18	0.43
1:S:11:GLN:OE1	1:S:11:GLN:HA	2.19	0.43
1:S:217:ARG:HH11	1:S:217:ARG:HG3	1.83	0.43
1:U:81:PHE:CZ	1:U:102:VAL:HG21	2.54	0.43
1:W:135:ARG:CB	1:W:135:ARG:HH11	2.32	0.43
2:E:475:ALA:HB3	3:E:20:DMF:H11	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:152:HIS:CG	1:M:171:TYR:CE2	3.07	0.43
2:R:394:ALA:HB1	2:R:399:LEU:HB2	2.01	0.43
1:Y:135:ARG:CB	1:Y:135:ARG:HH11	2.31	0.43
1:1:85:ARG:HD3	1:1:85:ARG:HA	1.87	0.43
2:E:388:ARG:NH1	5:E:2197:HOH:O	2.48	0.43
1:K:135:ARG:HH11	1:K:135:ARG:CB	2.32	0.43
1:O:213:LEU:HD23	1:O:213:LEU:HA	1.86	0.43
1:S:8:SER:N	1:S:11:GLN:HB2	2.29	0.43
1:S:181:LEU:HD23	1:S:233:LEU:HB3	2.00	0.43
2:Z:306:LEU:C	2:Z:306:LEU:HD12	2.39	0.43
1:A:52:LYS:HE2	1:A:64:ALA:O	2.18	0.43
1:I:52:LYS:HE2	1:I:64:ALA:O	2.18	0.43
1:I:73:ASN:ND2	1:S:105:GLN:OE1	2.52	0.43
2:L:456:GLN:HE22	2:L:465:ARG:HH22	1.67	0.43
1:O:167:LEU:C	1:O:169:GLU:N	2.70	0.43
1:Q:167:LEU:C	1:Q:169:GLU:N	2.71	0.43
1:S:142:THR:OG1	1:S:144:ASP:OD2	2.30	0.43
1:1:213:LEU:HA	1:1:213:LEU:HD23	1.87	0.43
1:B:33:LEU:HD12	1:B:33:LEU:O	2.19	0.43
1:I:178:THR:HG21	1:I:182:ARG:NH2	2.33	0.43
1:D:178:THR:CG2	1:D:182:ARG:HE	2.31	0.43
1:D:188:LEU:HB3	5:D:2659:HOH:O	2.18	0.43
1:D:19:LEU:HD23	1:D:19:LEU:O	2.19	0.43
1:F:178:THR:CG2	1:F:182:ARG:HE	2.31	0.43
4:H:300:SA6:O6	4:H:300:SA6:H1B	2.19	0.43
1:K:167:LEU:C	1:K:169:GLU:N	2.70	0.43
1:K:77:GLY:HA3	3:K:249:DMF:C	2.48	0.43
1:Q:81:PHE:CZ	1:Q:102:VAL:HG21	2.54	0.43
1:W:13:MET:O	1:W:17:SER:HB2	2.19	0.43
1:Y:217:ARG:HH11	1:Y:217:ARG:HG3	1.84	0.43
1:1:33:LEU:O	1:1:33:LEU:HD12	2.19	0.42
2:2:509:ARG:HG2	5:2:2190:HOH:O	2.19	0.42
1:B:97:ARG:NH2	5:B:1679:HOH:O	2.51	0.42
1:D:56:LEU:HD23	1:D:56:LEU:HA	1.86	0.42
1:I:162:PRO:CB	1:I:190:ALA:O	2.67	0.42
1:K:56:LEU:HG	1:K:62:PHE:HB2	2.00	0.42
2:P:436:TYR:CE1	3:P:107:DMF:H21	2.52	0.42
2:R:323:GLY:N	5:R:2674:HOH:O	2.47	0.42
5:J:1118:HOH:O	2:R:536:HIS:HE1	2.02	0.42
1:S:111:PHE:CE1	1:S:143:TYR:HE1	2.37	0.42
3:T:84:DMF:H11	5:T:2221:HOH:O	2.16	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:46:PRO:HA	1:W:207:SER:HA	2.01	0.42
1:W:45:ASN:OD1	1:W:46:PRO:HD2	2.19	0.42
1:Y:135:ARG:CB	1:Y:135:ARG:NH1	2.82	0.42
1:B:230:LEU:HD12	1:B:230:LEU:O	2.18	0.42
2:C:477:ASP:OD1	3:C:88:DMF:H23	2.19	0.42
2:C:377:ALA:O	3:C:47:DMF:H12	2.19	0.42
2:E:372:VAL:HG23	2:E:373:PRO:HD2	2.01	0.42
1:F:140:ARG:NH1	1:F:154:VAL:HG13	2.35	0.42
2:G:345:ILE:HB	2:G:352:ALA:HB1	2.00	0.42
1:M:169:GLU:OE1	1:M:169:GLU:CA	2.66	0.42
1:M:45:ASN:HA	1:M:46:PRO:HD2	1.91	0.42
5:J:594:HOH:O	1:S:85:ARG:HD2	2.19	0.42
1:S:90:ASP:HB3	1:S:93:ASP:OD2	2.19	0.42
1:W:170:SER:O	1:W:183:ILE:HD13	2.19	0.42
1:W:205:VAL:HG23	1:W:206:ALA:N	2.35	0.42
1:Y:174:ASN:HA	1:Y:174:ASN:HD22	1.64	0.42
1:Y:205:VAL:CG2	1:Y:206:ALA:N	2.81	0.42
2:N:511:ALA:O	2:N:515:ARG:HG3	2.19	0.42
1:Q:178:THR:CG2	1:Q:182:ARG:HE	2.31	0.42
1:U:52:LYS:HE2	1:U:64:ALA:O	2.19	0.42
1:I:45:ASN:HA	1:I:46:PRO:HD2	1.90	0.42
1:K:233:LEU:HD12	1:K:233:LEU:HA	1.93	0.42
1:M:142:THR:OG1	1:M:146:SER:HB2	2.20	0.42
1:O:81:PHE:CZ	1:O:102:VAL:HG21	2.54	0.42
2:G:447:LYS:HD3	3:G:119:DMF:C2	2.44	0.42
1:I:8:SER:N	1:I:11:GLN:HB2	2.34	0.42
1:W:178:THR:CG2	1:W:182:ARG:HE	2.31	0.42
2:Z:471:LEU:HD23	2:Z:471:LEU:HA	1.91	0.42
1:B:229:ALA:O	1:B:233:LEU:CD1	2.68	0.42
3:H:71:DMF:H21	5:P:1400:HOH:O	2.18	0.42
1:I:167:LEU:O	1:I:168:LYS:C	2.57	0.42
2:J:415:GLN:HG2	5:J:1219:HOH:O	2.18	0.42
1:K:81:PHE:CZ	1:K:102:VAL:HG21	2.54	0.42
1:K:28:LYS:HD2	1:K:44:GLU:OE2	2.20	0.42
1:M:90:ASP:HB3	1:M:93:ASP:OD2	2.20	0.42
1:O:228:SER:O	1:O:231:GLN:HB3	2.20	0.42
1:S:28:LYS:HG2	5:S:1910:HOH:O	2.19	0.42
1:W:135:ARG:NH1	1:W:135:ARG:CB	2.83	0.42
1:Y:52:LYS:CG	3:Y:251:DMF:HC	2.47	0.42
2:Z:366:TYR:CZ	2:Z:370:GLU:HG3	2.55	0.42
3:H:117:DMF:C	5:H:555:HOH:O	2.66	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:44:GLU:HG3	1:I:203:LEU:CD2	2.37	0.42
1:K:19:LEU:HD23	1:K:19:LEU:O	2.19	0.42
1:M:135:ARG:CB	1:M:135:ARG:HH11	2.32	0.42
1:O:19:LEU:C	1:O:19:LEU:HD23	2.40	0.42
1:W:11:GLN:O	1:W:14:ARG:HB3	2.19	0.42
1:W:182:ARG:NH2	1:W:234:LEU:O	2.52	0.42
1:Y:19:LEU:HD23	1:Y:19:LEU:O	2.20	0.42
1:Y:52:LYS:HE2	1:Y:64:ALA:O	2.20	0.42
2:Z:362:GLU:OE2	2:Z:382:ARG:NE	2.47	0.42
1:A:142:THR:OG1	1:A:146:SER:HB2	2.20	0.42
1:A:188:LEU:HA	1:A:188:LEU:HD12	1.84	0.42
2:C:435:GLY:HA2	2:R:530:ASP:OD1	2.20	0.42
2:G:393:ALA:HB1	2:G:398:LEU:HD12	2.01	0.42
1:I:233:LEU:CD1	5:I:1562:HOH:O	2.67	0.42
2:N:432:GLU:OE2	3:N:104:DMF:C2	2.52	0.42
2:X:444:LEU:HB2	5:X:2327:HOH:O	2.19	0.42
1:B:45:ASN:HA	1:B:46:PRO:HD2	1.89	0.42
1:D:167:LEU:C	1:D:169:GLU:N	2.70	0.42
1:K:135:ARG:NH1	1:K:135:ARG:CB	2.83	0.42
1:Q:45:ASN:HA	1:Q:46:PRO:HD2	1.91	0.42
2:R:306:LEU:O	2:R:306:LEU:HD12	2.20	0.42
1:A:8:SER:OG	1:A:11:GLN:HB2	2.19	0.42
1:D:144:ASP:OD2	1:D:146:SER:HB2	2.19	0.42
2:E:381:ASN:HB2	3:E:53:DMF:C1	2.39	0.42
2:G:447:LYS:CD	3:G:119:DMF:H22	2.46	0.42
1:M:217:ARG:HG3	1:M:217:ARG:HH11	1.85	0.42
1:M:85:ARG:HA	1:M:85:ARG:HD3	1.90	0.42
1:O:8:SER:O	1:O:9:PRO:C	2.59	0.42
2:R:325:MET:HE1	2:Z:444:LEU:HD11	2.02	0.42
3:2:108:DMF:H11	5:2:1666:HOH:O	2.20	0.41
5:T:1568:HOH:O	3:2:112:DMF:H21	2.18	0.41
1:B:135:ARG:CB	1:B:135:ARG:HH11	2.33	0.41
2:C:324:ASN:HB2	5:C:1419:HOH:O	2.19	0.41
2:G:444:LEU:HB2	3:G:64:DMF:H13	2.02	0.41
1:I:98:GLN:O	1:I:102:VAL:HG23	2.19	0.41
1:K:45:ASN:HA	1:K:46:PRO:HD2	1.88	0.41
2:T:362:GLU:OE2	2:T:382:ARG:HD2	2.18	0.41
1:U:161:GLU:CB	1:U:162:PRO:HD3	2.34	0.41
2:V:486:LEU:HB2	5:V:553:HOH:O	2.20	0.41
1:D:162:PRO:HB3	1:D:190:ALA:O	2.20	0.41
1:F:52:LYS:HE2	1:F:52:LYS:HB3	1.91	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:444:LEU:HB2	5:L:45:HOH:O	2.19	0.41
2:N:430:ASN:ND2	3:N:104:DMF:C	2.83	0.41
2:N:430:ASN:ND2	3:N:104:DMF:N	2.68	0.41
1:Q:56:LEU:HG	1:Q:62:PHE:HB2	2.01	0.41
1:Q:90:ASP:O	1:Q:93:ASP:HB2	2.20	0.41
1:Q:92:ARG:NH1	5:Q:1250:HOH:O	2.54	0.41
1:S:233:LEU:HD12	1:S:233:LEU:N	2.36	0.41
1:S:8:SER:OG	1:S:11:GLN:HB2	2.20	0.41
2:X:366:TYR:CZ	2:X:370:GLU:HG3	2.55	0.41
1:Y:81:PHE:CZ	1:Y:102:VAL:HG21	2.55	0.41
1:Y:181:LEU:O	1:Y:185:VAL:HG23	2.20	0.41
5:T:548:HOH:O	3:Z:94:DMF:H13	2.20	0.41
2:2:331:VAL:HG11	4:2:300:SA6:C19	2.47	0.41
2:J:461:ASP:OD1	2:J:509:ARG:NE	2.51	0.41
1:M:230:LEU:O	1:M:234:LEU:CD2	2.57	0.41
2:N:306:LEU:C	2:N:306:LEU:HD12	2.40	0.41
2:G:325:MET:SD	2:N:444:LEU:HD21	2.60	0.41
2:V:477:ASP:CG	3:V:120:DMF:H23	2.40	0.41
1:1:217:ARG:HG3	1:1:217:ARG:HH11	1.86	0.41
2:2:465:ARG:NH1	5:2:2328:HOH:O	2.37	0.41
1:D:81:PHE:CZ	1:D:102:VAL:HG21	2.56	0.41
2:E:301:THR:CG2	2:E:302:THR:N	2.84	0.41
1:F:225:ILE:HG21	1:F:233:LEU:CD1	2.50	0.41
1:I:166:ALA:O	1:I:170:SER:OG	2.36	0.41
1:I:205:VAL:HG12	1:I:230:LEU:HG	2.01	0.41
1:K:52:LYS:HB3	1:K:52:LYS:HE2	1.91	0.41
2:L:357:ARG:HD3	5:L:1243:HOH:O	2.21	0.41
1:M:22:LYS:HB3	1:M:26:ARG:HH21	1.85	0.41
1:O:203:LEU:CB	1:O:208:LEU:HD11	2.50	0.41
2:H:325:MET:SD	2:P:444:LEU:HD21	2.61	0.41
1:Q:85:ARG:HG2	5:Q:2261:HOH:O	2.20	0.41
3:V:83:DMF:H13	3:2:4:DMF:C	2.40	0.41
1:W:46:PRO:CD	1:W:47:SER:H	2.33	0.41
1:B:135:ARG:NH1	1:B:135:ARG:CB	2.84	0.41
1:B:217:ARG:HG3	1:B:217:ARG:HH11	1.86	0.41
1:K:85:ARG:NH2	5:K:2534:HOH:O	2.44	0.41
2:L:413:ASP:HA	2:L:414:PRO:HD3	1.88	0.41
2:P:447:LYS:CD	3:P:107:DMF:H23	2.49	0.41
2:R:496:ILE:HG13	2:R:505:VAL:CG2	2.50	0.41
1:W:85:ARG:HD3	1:W:85:ARG:HA	1.86	0.41
2:Z:413:ASP:HA	2:Z:414:PRO:HD3	1.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:90:ASP:HB3	1:1:93:ASP:OD2	2.20	0.41
2:C:409:ILE:HG23	5:C:2502:HOH:O	2.20	0.41
2:G:409:ILE:HG12	5:G:2516:HOH:O	2.20	0.41
1:I:19:LEU:HD11	1:S:13:MET:CG	2.51	0.41
2:J:516:ALA:CB	3:J:123:DMF:H12	2.46	0.41
2:J:383:LEU:HD23	2:J:423:PHE:CZ	2.56	0.41
2:P:413:ASP:HA	2:P:414:PRO:HD3	1.90	0.41
1:1:135:ARG:CB	1:1:135:ARG:HH11	2.34	0.41
2:2:492:PRO:O	2:2:510:ILE:HD13	2.20	0.41
2:H:447:LYS:HD2	3:H:43:DMF:C2	2.47	0.41
1:B:15:GLU:CD	1:I:8:SER:HB3	2.41	0.41
2:J:401:LEU:HD13	5:J:2229:HOH:O	2.20	0.41
2:L:440:GLY:HA2	3:L:97:DMF:C	2.51	0.41
1:U:213:LEU:HA	1:U:213:LEU:HD23	1.90	0.41
1:U:76:ARG:HD3	5:U:2597:HOH:O	2.20	0.41
2:V:429:TRP:CZ3	3:V:42:DMF:H13	2.56	0.41
2:Z:345:ILE:HD12	2:Z:352:ALA:O	2.21	0.41
2:G:372:VAL:HG23	2:G:373:PRO:HD2	2.03	0.41
2:H:331:VAL:HG11	4:H:300:SA6:C19	2.49	0.41
1:M:135:ARG:CB	1:M:135:ARG:NH1	2.83	0.41
1:O:135:ARG:CB	1:O:135:ARG:HH11	2.34	0.41
1:O:56:LEU:HA	1:O:56:LEU:HD23	1.86	0.41
1:Q:28:LYS:HD2	1:Q:44:GLU:OE2	2.21	0.41
1:W:40:LEU:CD1	1:W:212:VAL:HG12	2.50	0.41
1:W:40:LEU:HD12	1:W:212:VAL:HG12	2.03	0.41
2:X:483:GLY:HA3	3:X:122:DMF:H12	2.02	0.41
2:Z:345:ILE:HB	2:Z:352:ALA:HB1	2.02	0.41
2:2:306:LEU:HD12	2:2:306:LEU:C	2.41	0.41
1:I:107:LEU:HA	1:I:107:LEU:HD23	1.93	0.41
1:I:217:ARG:HH12	1:I:223:ARG:HD3	1.82	0.41
2:V:333:LYS:HG2	4:V:300:SA6:H18	2.03	0.41
2:2:476:ASP:OD1	3:2:49:DMF:H11	2.21	0.41
1:B:206:ALA:O	1:B:207:SER:CB	2.63	0.41
1:B:52:LYS:HE2	1:B:64:ALA:O	2.21	0.41
1:D:217:ARG:HG3	1:D:218:PRO:HD2	2.03	0.41
1:I:213:LEU:HD23	1:I:213:LEU:HA	1.84	0.41
1:D:15:GLU:CG	1:K:9:PRO:CG	2.98	0.41
1:O:7:ILE:CG2	1:O:8:SER:N	2.84	0.41
2:P:331:VAL:HG11	4:P:300:SA6:C19	2.49	0.41
1:Q:179:ASP:O	1:Q:183:ILE:HG13	2.21	0.41
1:U:135:ARG:CB	1:U:135:ARG:HH11	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:56:LEU:HD23	1:Y:56:LEU:HA	1.83	0.41
1:A:141:ILE:N	1:A:141:ILE:HD12	2.36	0.41
2:C:465:ARG:CD	5:C:1693:HOH:O	2.69	0.41
1:D:107:LEU:HD12	1:D:141:ILE:HG22	2.02	0.41
1:D:135:ARG:NH1	1:D:135:ARG:CB	2.84	0.41
1:K:85:ARG:HD2	5:K:254:HOH:O	2.20	0.41
1:K:98:GLN:O	1:K:102:VAL:HG23	2.21	0.41
3:N:22:DMF:C	5:N:2569:HOH:O	2.44	0.41
2:P:345:ILE:HB	2:P:352:ALA:HB1	2.03	0.41
2:R:444:LEU:HB2	3:R:59:DMF:N	2.35	0.41
1:U:129:HIS:O	1:U:132:GLU:HB3	2.21	0.41
1:U:135:ARG:CB	1:U:135:ARG:NH1	2.84	0.41
1:I:135:ARG:CB	1:I:135:ARG:NH1	2.85	0.40
1:A:33:LEU:O	1:A:33:LEU:HD12	2.21	0.40
1:D:135:ARG:HH11	1:D:135:ARG:CB	2.33	0.40
1:F:167:LEU:O	1:F:168:LYS:C	2.57	0.40
1:I:205:VAL:HG23	1:I:206:ALA:N	2.35	0.40
1:I:28:LYS:HD2	1:I:44:GLU:OE2	2.21	0.40
1:K:205:VAL:HG23	1:K:206:ALA:N	2.36	0.40
1:M:114:GLN:HB3	1:M:114:GLN:HE21	1.59	0.40
1:Q:135:ARG:CB	1:Q:135:ARG:HH11	2.34	0.40
1:D:105:GLN:OE1	1:Q:73:ASN:ND2	2.53	0.40
1:S:163:ILE:HD13	1:S:188:LEU:HD12	2.03	0.40
2:T:464:LEU:HG	2:T:513:LEU:CD1	2.50	0.40
1:U:95:THR:OG1	1:U:98:GLN:HG3	2.21	0.40
1:I:141:ILE:HD12	1:I:141:ILE:N	2.36	0.40
1:A:233:LEU:N	1:A:233:LEU:HD12	2.36	0.40
2:C:465:ARG:HD2	5:C:1693:HOH:O	2.20	0.40
1:F:90:ASP:HB3	1:F:93:ASP:OD2	2.20	0.40
1:I:217:ARG:NH1	1:I:223:ARG:CD	2.77	0.40
2:J:515:ARG:HH12	2:R:539:HIS:N	2.16	0.40
1:M:181:LEU:HD23	1:M:233:LEU:HB3	2.03	0.40
1:O:217:ARG:HH11	1:O:217:ARG:HG3	1.86	0.40
1:I:163:ILE:HD13	1:I:188:LEU:HD12	2.02	0.40
1:A:135:ARG:CB	1:A:135:ARG:HH11	2.34	0.40
1:A:217:ARG:HG3	1:A:217:ARG:HH11	1.86	0.40
1:D:144:ASP:CG	1:D:146:SER:OG	2.60	0.40
3:D:253:DMF:H13	2:E:361:VAL:HG11	2.02	0.40
1:K:56:LEU:HD23	1:K:56:LEU:HA	1.82	0.40
1:M:76:ARG:HD3	5:M:1491:HOH:O	2.21	0.40
2:N:362:GLU:OE2	2:N:382:ARG:HD2	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:415:GLN:NE2	5:P:2154:HOH:O	2.43	0.40
1:U:233:LEU:HD12	1:U:233:LEU:N	2.36	0.40
1:W:45:ASN:N	1:W:207:SER:O	2.54	0.40
1:Q:105:GLN:OE1	1:Y:73:ASN:ND2	2.55	0.40
3:T:113:DMF:H12	3:2:112:DMF:H21	2.03	0.40
1:D:52:LYS:HB3	1:D:52:LYS:HE2	1.89	0.40
2:E:432:GLU:OE2	2:E:434:GLU:HB2	2.21	0.40
2:E:461:ASP:CG	2:E:509:ARG:HH21	2.23	0.40
1:F:8:SER:HB2	1:F:9:PRO:HD2	2.03	0.40
1:O:135:ARG:NH1	1:O:135:ARG:CB	2.85	0.40
4:R:300:SA6:O6	4:R:300:SA6:H1B	2.21	0.40
2:T:413:ASP:HA	2:T:414:PRO:HD3	1.89	0.40
1:W:167:LEU:HG	1:W:187:ALA:HB1	2.02	0.40
1:I:11:GLN:HE21	1:I:11:GLN:CA	2.26	0.40
1:A:98:GLN:O	1:A:102:VAL:HG23	2.21	0.40
1:I:233:LEU:H	1:I:233:LEU:HD12	1.87	0.40
1:I:52:LYS:HE2	1:I:52:LYS:HB3	1.90	0.40
1:I:97:ARG:NE	5:I:2433:HOH:O	2.52	0.40
2:J:306:LEU:C	2:J:306:LEU:HD12	2.41	0.40
1:K:213:LEU:HD23	1:K:213:LEU:HA	1.86	0.40
1:K:52:LYS:HE2	1:K:64:ALA:O	2.22	0.40
1:M:182:ARG:NH1	1:M:234:LEU:O	2.55	0.40
2:N:432:GLU:CD	2:N:437:GLN:HE21	2.25	0.40
1:Q:16:ARG:NH2	1:Q:115:ALA:O	2.54	0.40
1:S:85:ARG:CD	1:S:89:TYR:CD2	3.04	0.40

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%)	199 (94%)	12 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	211/248 (85%)	203 (96%)	8 (4%)	0	100	100
1	B	209/248 (84%)	201 (96%)	8 (4%)	0	100	100
1	D	210/248 (85%)	201 (96%)	9 (4%)	0	100	100
1	F	216/248 (87%)	209 (97%)	6 (3%)	1 (0%)	32	34
1	I	212/248 (86%)	201 (95%)	11 (5%)	0	100	100
1	K	212/248 (86%)	202 (95%)	10 (5%)	0	100	100
1	M	212/248 (86%)	201 (95%)	11 (5%)	0	100	100
1	O	212/248 (86%)	199 (94%)	13 (6%)	0	100	100
1	Q	211/248 (85%)	198 (94%)	13 (6%)	0	100	100
1	S	212/248 (86%)	203 (96%)	9 (4%)	0	100	100
1	U	212/248 (86%)	200 (94%)	12 (6%)	0	100	100
1	W	212/248 (86%)	199 (94%)	13 (6%)	0	100	100
1	Y	212/248 (86%)	202 (95%)	10 (5%)	0	100	100
2	2	221/240 (92%)	220 (100%)	1 (0%)	0	100	100
2	C	220/240 (92%)	219 (100%)	1 (0%)	0	100	100
2	E	221/240 (92%)	219 (99%)	2 (1%)	0	100	100
2	G	220/240 (92%)	218 (99%)	2 (1%)	0	100	100
2	H	220/240 (92%)	219 (100%)	1 (0%)	0	100	100
2	J	220/240 (92%)	219 (100%)	1 (0%)	0	100	100
2	L	221/240 (92%)	218 (99%)	3 (1%)	0	100	100
2	N	220/240 (92%)	218 (99%)	2 (1%)	0	100	100
2	P	220/240 (92%)	218 (99%)	2 (1%)	0	100	100
2	R	237/240 (99%)	236 (100%)	1 (0%)	0	100	100
2	T	221/240 (92%)	220 (100%)	1 (0%)	0	100	100
2	V	237/240 (99%)	234 (99%)	3 (1%)	0	100	100
2	X	221/240 (92%)	219 (99%)	2 (1%)	0	100	100
2	Z	221/240 (92%)	218 (99%)	3 (1%)	0	100	100
All	All	6084/6832 (89%)	5913 (97%)	170 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	191	GLY

### 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	165/192 (86%)	158 (96%)	7 (4%)	34	43
1	A	164/192 (85%)	155 (94%)	9 (6%)	25	29
1	B	163/192 (85%)	154 (94%)	9 (6%)	25	29
1	D	164/192 (85%)	152 (93%)	12 (7%)	16	17
1	F	169/192 (88%)	161 (95%)	8 (5%)	30	37
1	I	166/192 (86%)	161 (97%)	5 (3%)	46	58
1	K	166/192 (86%)	157 (95%)	9 (5%)	26	30
1	M	166/192 (86%)	155 (93%)	11 (7%)	19	21
1	O	166/192 (86%)	161 (97%)	5 (3%)	46	58
1	Q	165/192 (86%)	158 (96%)	7 (4%)	34	43
1	S	166/192 (86%)	158 (95%)	8 (5%)	30	36
1	U	165/192 (86%)	160 (97%)	5 (3%)	46	58
1	W	166/192 (86%)	160 (96%)	6 (4%)	40	50
1	Y	166/192 (86%)	159 (96%)	7 (4%)	34	43
2	2	165/178 (93%)	160 (97%)	5 (3%)	46	58
2	C	165/178 (93%)	163 (99%)	2 (1%)	75	86
2	E	165/178 (93%)	161 (98%)	4 (2%)	54	67
2	G	165/178 (93%)	163 (99%)	2 (1%)	75	86
2	H	165/178 (93%)	162 (98%)	3 (2%)	64	77
2	J	165/178 (93%)	161 (98%)	4 (2%)	54	67
2	L	165/178 (93%)	160 (97%)	5 (3%)	46	58
2	N	165/178 (93%)	162 (98%)	3 (2%)	64	77
2	P	165/178 (93%)	163 (99%)	2 (1%)	75	86
2	R	177/178 (99%)	173 (98%)	4 (2%)	56	69
2	T	165/178 (93%)	160 (97%)	5 (3%)	46	58
2	V	177/178 (99%)	173 (98%)	4 (2%)	56	69

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	X	165/178 (93%)	162 (98%)	3 (2%)	64	77
2	Z	165/178 (93%)	162 (98%)	3 (2%)	64	77
All	All	4651/5180 (90%)	4494 (97%)	157 (3%)	42	53

All (157) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	LEU
1	A	69	ASN
1	A	73	ASN
1	A	74	LEU
1	A	80	GLN
1	A	173	GLU
1	A	182	ARG
1	A	188	LEU
1	A	234	LEU
1	B	7	ILE
1	B	14	ARG
1	B	21	ARG
1	B	33	LEU
1	B	69	ASN
1	B	73	ASN
1	B	74	LEU
1	B	182	ARG
1	B	233	LEU
2	C	363	LEU
2	C	444	LEU
1	D	10	GLU
1	D	33	LEU
1	D	69	ASN
1	D	73	ASN
1	D	74	LEU
1	D	144	ASP
1	D	147	ILE
1	D	170	SER
1	D	174	ASN
1	D	182	ARG
1	D	205	VAL
1	D	208	LEU
2	E	354	GLU
2	E	363	LEU

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Mol	Chain	Res	Type
2	E	434	GLU
2	E	444	LEU
1	F	5	TYR
1	F	33	LEU
1	F	69	ASN
1	F	73	ASN
1	F	74	LEU
1	F	173	GLU
1	F	182	ARG
1	F	203	LEU
2	G	363	LEU
2	G	444	LEU
2	H	363	LEU
2	H	433	GLU
2	H	444	LEU
1	I	33	LEU
1	I	69	ASN
1	I	73	ASN
1	I	74	LEU
1	I	114	GLN
2	J	363	LEU
2	J	396	GLN
2	J	398	LEU
2	J	444	LEU
1	K	7	ILE
1	K	11	GLN
1	K	33	LEU
1	K	69	ASN
1	K	73	ASN
1	K	74	LEU
1	K	174	ASN
1	K	182	ARG
1	K	189	ARG
2	L	363	LEU
2	L	432	GLU
2	L	444	LEU
2	L	459	ASP
2	L	509	ARG
1	M	10	GLU
1	M	26	ARG
1	M	33	LEU
1	M	69	ASN

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Mol	Chain	Res	Type
1	M	73	ASN
1	M	74	LEU
1	M	169	GLU
1	M	182	ARG
1	M	203	LEU
1	M	205	VAL
1	M	234	LEU
2	N	363	LEU
2	N	444	LEU
2	N	512	GLU
1	O	33	LEU
1	O	69	ASN
1	O	73	ASN
1	O	74	LEU
1	O	182	ARG
2	P	363	LEU
2	P	444	LEU
1	Q	33	LEU
1	Q	69	ASN
1	Q	73	ASN
1	Q	74	LEU
1	Q	114	GLN
1	Q	174	ASN
1	Q	182	ARG
2	R	363	LEU
2	R	433	GLU
2	R	444	LEU
2	R	538	HIS
1	S	7	ILE
1	S	11	GLN
1	S	33	LEU
1	S	69	ASN
1	S	73	ASN
1	S	74	LEU
1	S	182	ARG
1	S	205	VAL
2	T	363	LEU
2	T	398	LEU
2	T	444	LEU
2	T	486	LEU
2	T	509	ARG
1	U	7	ILE

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Mol	Chain	Res	Type
1	U	33	LEU
1	U	69	ASN
1	U	73	ASN
1	U	74	LEU
2	V	363	LEU
2	V	433	GLU
2	V	444	LEU
2	V	538	HIS
1	W	7	ILE
1	W	33	LEU
1	W	69	ASN
1	W	92	ARG
1	W	142	THR
1	W	182	ARG
2	X	363	LEU
2	X	444	LEU
2	X	519	GLU
1	Y	33	LEU
1	Y	69	ASN
1	Y	73	ASN
1	Y	74	LEU
1	Y	173	GLU
1	Y	182	ARG
1	Y	203	LEU
2	Z	363	LEU
2	Z	444	LEU
2	Z	519	GLU
1	1	33	LEU
1	1	69	ASN
1	1	73	ASN
1	1	74	LEU
1	1	174	ASN
1	1	182	ARG
1	1	234	LEU
2	2	363	LEU
2	2	433	GLU
2	2	444	LEU
2	2	465	ARG
2	2	512	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (92) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	69	ASN
1	A	80	GLN
1	A	114	GLN
1	A	129	HIS
1	B	69	ASN
1	B	80	GLN
1	B	174	ASN
2	C	456	GLN
1	D	69	ASN
1	D	73	ASN
1	D	80	GLN
1	D	98	GLN
1	D	114	GLN
1	D	152	HIS
1	D	174	ASN
2	E	430	ASN
2	E	456	GLN
1	F	69	ASN
1	F	73	ASN
1	F	80	GLN
1	F	114	GLN
2	G	430	ASN
2	G	456	GLN
2	H	456	GLN
1	I	69	ASN
1	I	73	ASN
1	I	80	GLN
1	I	114	GLN
1	I	129	HIS
2	J	322	GLN
2	J	430	ASN
2	J	456	GLN
1	K	11	GLN
1	K	69	ASN
1	K	80	GLN
2	L	430	ASN
2	L	456	GLN
1	M	11	GLN
1	M	69	ASN
1	M	80	GLN
1	M	114	GLN
1	M	129	HIS
2	N	430	ASN

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Mol	Chain	Res	Type
2	N	456	GLN
1	O	69	ASN
1	O	73	ASN
1	O	80	GLN
1	O	114	GLN
2	P	430	ASN
2	P	456	GLN
1	Q	69	ASN
1	Q	73	ASN
1	Q	80	GLN
1	Q	174	ASN
2	R	430	ASN
2	R	456	GLN
2	R	536	HIS
2	R	538	HIS
1	S	69	ASN
1	S	73	ASN
1	S	80	GLN
1	S	114	GLN
1	S	129	HIS
1	S	152	HIS
2	T	456	GLN
1	U	69	ASN
1	U	80	GLN
1	U	114	GLN
1	U	129	HIS
1	U	231	GLN
2	V	430	ASN
2	V	456	GLN
2	V	538	HIS
1	W	69	ASN
1	W	80	GLN
1	W	114	GLN
1	W	129	HIS
2	X	430	ASN
2	X	456	GLN
1	Y	69	ASN
1	Y	73	ASN
1	Y	80	GLN
1	Y	114	GLN
1	Y	174	ASN
2	Z	430	ASN

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Mol	Chain	Res	Type
2	Z	456	GLN
1	1	11	GLN
1	1	69	ASN
1	1	80	GLN
1	1	114	GLN
2	2	430	ASN
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 ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

137 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	0.29	0	4,4,4	0.35	0
3	DMF	2	101	-	4,4,4	0.33	0	4,4,4	0.39	0
3	DMF	2	108	-	4,4,4	0.31	0	4,4,4	0.42	0
3	DMF	2	112	-	4,4,4	0.18	0	4,4,4	0.37	0
4	SA6	2	300	2	17,21,21	2.40	5 (29%)	21,32,32	1.85	7 (33%)
3	DMF	2	4	-	4,4,4	0.32	0	4,4,4	0.44	0
3	DMF	2	49	-	4,4,4	0.25	0	4,4,4	0.47	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	DMF	2	52	-	4,4,4	0.32	0	4,4,4	0.40	0
3	DMF	2	57	-	4,4,4	0.31	0	4,4,4	0.31	0
3	DMF	2	87	-	4,4,4	0.30	0	4,4,4	0.41	0
3	DMF	A	249	-	4,4,4	0.58	0	4,4,4	0.27	0
3	DMF	A	250	-	4,4,4	0.47	0	4,4,4	0.49	0
3	DMF	B	249	-	4,4,4	0.28	0	4,4,4	0.39	0
3	DMF	B	250	-	4,4,4	0.29	0	4,4,4	0.33	0
3	DMF	C	103	-	4,4,4	0.31	0	4,4,4	0.34	0
3	DMF	C	121	-	4,4,4	0.30	0	4,4,4	0.41	0
4	SA6	C	300	2	17,21,21	2.88	6 (35%)	21,32,32	1.93	6 (28%)
3	DMF	C	38	-	4,4,4	0.18	0	4,4,4	0.49	0
3	DMF	C	47	-	4,4,4	0.55	0	4,4,4	0.22	0
3	DMF	C	63	-	4,4,4	0.28	0	4,4,4	0.49	0
3	DMF	C	69	-	4,4,4	0.29	0	4,4,4	0.43	0
3	DMF	C	88	-	4,4,4	0.32	0	4,4,4	0.47	0
3	DMF	D	249	-	4,4,4	0.58	0	4,4,4	0.34	0
3	DMF	D	250	-	4,4,4	0.33	0	4,4,4	0.37	0
3	DMF	D	251	-	4,4,4	0.30	0	4,4,4	0.39	0
3	DMF	D	252	-	4,4,4	0.29	0	4,4,4	0.37	0
3	DMF	D	253	-	4,4,4	0.27	0	4,4,4	0.31	0
3	DMF	E	100	-	4,4,4	0.31	0	4,4,4	0.44	0
3	DMF	E	20	-	4,4,4	0.31	0	4,4,4	0.42	0
3	DMF	E	28	-	4,4,4	0.29	0	4,4,4	0.20	0
4	SA6	E	300	2	17,21,21	2.83	8 (47%)	21,32,32	1.80	5 (23%)
3	DMF	E	53	-	4,4,4	0.30	0	4,4,4	0.38	0
3	DMF	E	73	-	4,4,4	0.28	0	4,4,4	0.41	0
3	DMF	E	75	-	4,4,4	0.28	0	4,4,4	0.39	0
3	DMF	F	249	-	4,4,4	0.27	0	4,4,4	0.36	0
3	DMF	F	250	-	4,4,4	0.29	0	4,4,4	0.34	0
3	DMF	F	251	-	4,4,4	0.20	0	4,4,4	0.37	0
3	DMF	G	111	-	4,4,4	0.25	0	4,4,4	0.33	0
3	DMF	G	119	-	4,4,4	0.28	0	4,4,4	0.33	0
3	DMF	G	12	-	4,4,4	0.29	0	4,4,4	0.41	0
3	DMF	G	24	-	4,4,4	0.30	0	4,4,4	0.38	0
4	SA6	G	300	2	17,21,21	3.01	7 (41%)	21,32,32	1.52	2 (9%)
3	DMF	G	62	-	4,4,4	0.30	0	4,4,4	0.39	0
3	DMF	G	64	-	4,4,4	0.31	0	4,4,4	0.35	0
3	DMF	G	70	-	4,4,4	0.70	0	4,4,4	0.30	0
3	DMF	G	77	-	4,4,4	0.44	0	4,4,4	0.40	0
3	DMF	G	98	-	4,4,4	0.31	0	4,4,4	0.39	0
3	DMF	H	117	-	4,4,4	0.40	0	4,4,4	0.76	0
4	SA6	H	300	2	17,21,21	3.05	8 (47%)	21,32,32	1.62	5 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	DMF	H	43	-	4,4,4	0.37	0	4,4,4	0.70	0
3	DMF	H	66	-	4,4,4	0.30	0	4,4,4	0.40	0
3	DMF	H	71	-	4,4,4	0.51	0	4,4,4	0.36	0
3	DMF	H	72	-	4,4,4	0.32	0	4,4,4	0.39	0
3	DMF	H	91	-	4,4,4	0.29	0	4,4,4	0.43	0
3	DMF	I	249	-	4,4,4	0.32	0	4,4,4	0.38	0
3	DMF	I	250	-	4,4,4	0.28	0	4,4,4	0.32	0
3	DMF	J	110	-	4,4,4	0.34	0	4,4,4	0.57	0
3	DMF	J	123	-	4,4,4	0.30	0	4,4,4	0.39	0
4	SA6	J	300	2	17,21,21	3.18	9 (52%)	21,32,32	1.54	4 (19%)
3	DMF	J	45	-	4,4,4	0.29	0	4,4,4	0.30	0
3	DMF	K	249	-	4,4,4	0.29	0	4,4,4	0.37	0
3	DMF	K	250	-	4,4,4	0.27	0	4,4,4	0.32	0
3	DMF	K	251	-	4,4,4	0.31	0	4,4,4	0.16	0
3	DMF	K	252	-	4,4,4	0.28	0	4,4,4	0.35	0
4	SA6	L	300	2	17,21,21	3.20	8 (47%)	21,32,32	1.90	6 (28%)
3	DMF	L	36	-	4,4,4	0.32	0	4,4,4	0.44	0
3	DMF	L	50	-	4,4,4	0.23	0	4,4,4	0.27	0
3	DMF	L	81	-	4,4,4	0.29	0	4,4,4	0.31	0
3	DMF	L	97	-	4,4,4	0.30	0	4,4,4	0.41	0
3	DMF	M	249	-	4,4,4	0.30	0	4,4,4	0.41	0
3	DMF	M	250	-	4,4,4	0.31	0	4,4,4	0.34	0
3	DMF	M	251	-	4,4,4	0.31	0	4,4,4	0.31	0
3	DMF	M	252	-	4,4,4	0.33	0	4,4,4	0.36	0
3	DMF	N	104	-	4,4,4	0.34	0	4,4,4	0.38	0
3	DMF	N	118	-	4,4,4	0.37	0	4,4,4	0.63	0
3	DMF	N	22	-	4,4,4	0.31	0	4,4,4	0.34	0
4	SA6	N	300	2	17,21,21	2.67	7 (41%)	21,32,32	1.69	5 (23%)
3	DMF	N	90	-	4,4,4	0.30	0	4,4,4	0.43	0
3	DMF	N	93	-	4,4,4	0.32	0	4,4,4	0.38	0
3	DMF	O	249	-	4,4,4	0.25	0	4,4,4	0.50	0
3	DMF	O	250	-	4,4,4	0.34	0	4,4,4	0.37	0
3	DMF	O	251	-	4,4,4	0.40	0	4,4,4	0.76	0
3	DMF	P	107	-	4,4,4	0.23	0	4,4,4	0.42	0
3	DMF	P	14	-	4,4,4	0.28	0	4,4,4	0.39	0
3	DMF	P	2	-	4,4,4	0.28	0	4,4,4	0.50	0
4	SA6	P	300	2	17,21,21	2.84	7 (41%)	21,32,32	1.71	4 (19%)
3	DMF	P	33	-	4,4,4	0.28	0	4,4,4	0.23	0
3	DMF	P	51	-	4,4,4	0.26	0	4,4,4	0.33	0
3	DMF	P	56	-	4,4,4	0.30	0	4,4,4	0.42	0
3	DMF	P	60	-	4,4,4	0.28	0	4,4,4	0.38	0
3	DMF	P	86	-	4,4,4	0.29	0	4,4,4	0.38	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	DMF	Q	249	-	4,4,4	0.30	0	4,4,4	0.38	0
3	DMF	Q	250	-	4,4,4	0.27	0	4,4,4	0.51	0
3	DMF	Q	251	-	4,4,4	0.31	0	4,4,4	0.33	0
4	SA6	R	300	2	17,21,21	3.63	7 (41%)	21,32,32	1.74	5 (23%)
3	DMF	R	59	-	4,4,4	0.31	0	4,4,4	0.38	0
3	DMF	R	80	-	4,4,4	0.29	0	4,4,4	0.36	0
3	DMF	R	89	-	4,4,4	0.40	0	4,4,4	0.65	0
3	DMF	R	92	-	4,4,4	0.29	0	4,4,4	0.38	0
3	DMF	R	95	-	4,4,4	0.34	0	4,4,4	0.36	0
3	DMF	S	249	-	4,4,4	0.29	0	4,4,4	0.34	0
3	DMF	S	250	-	4,4,4	0.68	0	4,4,4	0.34	0
3	DMF	T	10	-	4,4,4	0.34	0	4,4,4	0.49	0
3	DMF	T	102	-	4,4,4	0.16	0	4,4,4	0.13	0
3	DMF	T	113	-	4,4,4	0.24	0	4,4,4	0.41	0
3	DMF	T	115	-	4,4,4	0.32	0	4,4,4	0.47	0
3	DMF	T	29	-	4,4,4	0.29	0	4,4,4	0.37	0
4	SA6	T	300	2	17,21,21	3.09	7 (41%)	21,32,32	1.82	4 (19%)
3	DMF	T	84	-	4,4,4	0.08	0	4,4,4	0.15	0
3	DMF	U	249	-	4,4,4	0.29	0	4,4,4	0.32	0
3	DMF	U	250	-	4,4,4	0.68	0	4,4,4	0.31	0
3	DMF	V	109	-	4,4,4	0.22	0	4,4,4	0.29	0
3	DMF	V	116	-	4,4,4	0.44	0	4,4,4	1.00	0
3	DMF	V	120	-	4,4,4	0.34	0	4,4,4	0.42	0
3	DMF	V	27	-	4,4,4	0.30	0	4,4,4	0.33	0
4	SA6	V	300	2	17,21,21	3.05	8 (47%)	21,32,32	1.43	3 (14%)
3	DMF	V	32	-	4,4,4	0.31	0	4,4,4	0.45	0
3	DMF	V	39	-	4,4,4	0.32	0	4,4,4	0.36	0
3	DMF	V	42	-	4,4,4	0.29	0	4,4,4	0.45	0
3	DMF	V	82	-	4,4,4	0.34	0	4,4,4	0.40	0
3	DMF	V	83	-	4,4,4	0.24	0	4,4,4	0.40	0
3	DMF	W	249	-	4,4,4	0.30	0	4,4,4	0.39	0
3	DMF	W	250	-	4,4,4	0.29	0	4,4,4	0.42	0
3	DMF	X	122	-	4,4,4	0.30	0	4,4,4	0.33	0
3	DMF	X	15	-	4,4,4	0.31	0	4,4,4	0.44	0
3	DMF	X	16	-	4,4,4	0.28	0	4,4,4	0.38	0
4	SA6	X	300	2	17,21,21	3.10	9 (52%)	21,32,32	1.64	1 (4%)
3	DMF	X	40	-	4,4,4	0.32	0	4,4,4	0.39	0
3	DMF	X	41	-	4,4,4	0.55	0	4,4,4	0.34	0
3	DMF	Y	249	-	4,4,4	0.31	0	4,4,4	0.40	0
3	DMF	Y	250	-	4,4,4	0.65	0	4,4,4	0.31	0
3	DMF	Y	251	-	4,4,4	0.31	0	4,4,4	0.40	0
3	DMF	Z	114	-	4,4,4	0.33	0	4,4,4	0.43	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	DMF	Z	18	-	4,4,4	0.23	0	4,4,4	0.40	0
4	SA6	Z	300	2	17,21,21	3.28	11 (64%)	21,32,32	1.56	3 (14%)
3	DMF	Z	54	-	4,4,4	0.34	0	4,4,4	0.45	0
3	DMF	Z	94	-	4,4,4	0.27	0	4,4,4	0.37	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	2	101	-	-	0/2/2/2	0/0/0/0
3	DMF	2	108	-	-	0/2/2/2	0/0/0/0
3	DMF	2	112	-	-	0/2/2/2	0/0/0/0
4	SA6	2	300	2	-	0/6/47/47	0/2/2/2
3	DMF	2	4	-	-	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	57	-	-	0/2/2/2	0/0/0/0
3	DMF	2	87	-	-	0/2/2/2	0/0/0/0
3	DMF	A	249	-	-	0/2/2/2	0/0/0/0
3	DMF	A	250	-	-	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	103	-	-	0/2/2/2	0/0/0/0
3	DMF	C	121	-	-	0/2/2/2	0/0/0/0
4	SA6	C	300	2	-	0/6/47/47	0/2/2/2
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	63	-	-	0/2/2/2	0/0/0/0
3	DMF	C	69	-	-	0/2/2/2	0/0/0/0
3	DMF	C	88	-	-	0/2/2/2	0/0/0/0
3	DMF	D	249	-	-	0/2/2/2	0/0/0/0
3	DMF	D	250	-	-	0/2/2/2	0/0/0/0
3	DMF	D	251	-	-	0/2/2/2	0/0/0/0
3	DMF	D	252	-	-	0/2/2/2	0/0/0/0
3	DMF	D	253	-	-	0/2/2/2	0/0/0/0
3	DMF	E	100	-	-	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
4	SA6	E	300	2	-	0/6/47/47	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	DMF	E	53	-	-	0/2/2/2	0/0/0/0
3	DMF	E	73	-	-	0/2/2/2	0/0/0/0
3	DMF	E	75	-	-	0/2/2/2	0/0/0/0
3	DMF	F	249	-	-	0/2/2/2	0/0/0/0
3	DMF	F	250	-	-	0/2/2/2	0/0/0/0
3	DMF	F	251	-	-	0/2/2/2	0/0/0/0
3	DMF	G	111	-	-	0/2/2/2	0/0/0/0
3	DMF	G	119	-	-	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
4	SA6	G	300	2	-	0/6/47/47	0/2/2/2
3	DMF	G	62	-	-	0/2/2/2	0/0/0/0
3	DMF	G	64	-	-	0/2/2/2	0/0/0/0
3	DMF	G	70	-	-	0/2/2/2	0/0/0/0
3	DMF	G	77	-	-	0/2/2/2	0/0/0/0
3	DMF	G	98	-	-	0/2/2/2	0/0/0/0
3	DMF	H	117	-	-	0/2/2/2	0/0/0/0
4	SA6	H	300	2	-	0/6/47/47	0/2/2/2
3	DMF	H	43	-	-	0/2/2/2	0/0/0/0
3	DMF	H	66	-	-	0/2/2/2	0/0/0/0
3	DMF	H	71	-	-	0/2/2/2	0/0/0/0
3	DMF	H	72	-	-	0/2/2/2	0/0/0/0
3	DMF	H	91	-	-	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	110	-	-	0/2/2/2	0/0/0/0
3	DMF	J	123	-	-	0/2/2/2	0/0/0/0
4	SA6	J	300	2	-	0/6/47/47	0/2/2/2
3	DMF	J	45	-	-	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	K	252	-	-	0/2/2/2	0/0/0/0
4	SA6	L	300	2	-	0/6/47/47	0/2/2/2
3	DMF	L	36	-	-	0/2/2/2	0/0/0/0
3	DMF	L	50	-	-	0/2/2/2	0/0/0/0
3	DMF	L	81	-	-	0/2/2/2	0/0/0/0
3	DMF	L	97	-	-	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	M	251	-	-	0/2/2/2	0/0/0/0
3	DMF	M	252	-	-	0/2/2/2	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	DMF	N	104	-	-	0/2/2/2	0/0/0/0
3	DMF	N	118	-	-	0/2/2/2	0/0/0/0
3	DMF	N	22	-	-	0/2/2/2	0/0/0/0
4	SA6	N	300	2	-	0/6/47/47	0/2/2/2
3	DMF	N	90	-	-	0/2/2/2	0/0/0/0
3	DMF	N	93	-	-	0/2/2/2	0/0/0/0
3	DMF	O	249	-	-	0/2/2/2	0/0/0/0
3	DMF	O	250	-	-	0/2/2/2	0/0/0/0
3	DMF	O	251	-	-	0/2/2/2	0/0/0/0
3	DMF	P	107	-	-	0/2/2/2	0/0/0/0
3	DMF	P	14	-	-	0/2/2/2	0/0/0/0
3	DMF	P	2	-	-	0/2/2/2	0/0/0/0
4	SA6	P	300	2	-	0/6/47/47	0/2/2/2
3	DMF	P	33	-	-	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	60	-	-	0/2/2/2	0/0/0/0
3	DMF	P	86	-	-	0/2/2/2	0/0/0/0
3	DMF	Q	249	-	-	0/2/2/2	0/0/0/0
3	DMF	Q	250	-	-	0/2/2/2	0/0/0/0
3	DMF	Q	251	-	-	0/2/2/2	0/0/0/0
4	SA6	R	300	2	-	0/6/47/47	0/2/2/2
3	DMF	R	59	-	-	0/2/2/2	0/0/0/0
3	DMF	R	80	-	-	0/2/2/2	0/0/0/0
3	DMF	R	89	-	-	0/2/2/2	0/0/0/0
3	DMF	R	92	-	-	0/2/2/2	0/0/0/0
3	DMF	R	95	-	-	0/2/2/2	0/0/0/0
3	DMF	S	249	-	-	0/2/2/2	0/0/0/0
3	DMF	S	250	-	-	0/2/2/2	0/0/0/0
3	DMF	T	10	-	-	0/2/2/2	0/0/0/0
3	DMF	T	102	-	-	0/2/2/2	0/0/0/0
3	DMF	T	113	-	-	0/2/2/2	0/0/0/0
3	DMF	T	115	-	-	0/2/2/2	0/0/0/0
3	DMF	T	29	-	-	0/2/2/2	0/0/0/0
4	SA6	T	300	2	-	0/6/47/47	0/2/2/2
3	DMF	T	84	-	-	0/2/2/2	0/0/0/0
3	DMF	U	249	-	-	0/2/2/2	0/0/0/0
3	DMF	U	250	-	-	0/2/2/2	0/0/0/0
3	DMF	V	109	-	-	0/2/2/2	0/0/0/0
3	DMF	V	116	-	-	0/2/2/2	0/0/0/0
3	DMF	V	120	-	-	0/2/2/2	0/0/0/0
3	DMF	V	27	-	-	0/2/2/2	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	SA6	V	300	2	-	0/6/47/47	0/2/2/2
3	DMF	V	32	-	-	0/2/2/2	0/0/0/0
3	DMF	V	39	-	-	0/2/2/2	0/0/0/0
3	DMF	V	42	-	-	0/2/2/2	0/0/0/0
3	DMF	V	82	-	-	0/2/2/2	0/0/0/0
3	DMF	V	83	-	-	0/2/2/2	0/0/0/0
3	DMF	W	249	-	-	0/2/2/2	0/0/0/0
3	DMF	W	250	-	-	0/2/2/2	0/0/0/0
3	DMF	X	122	-	-	0/2/2/2	0/0/0/0
3	DMF	X	15	-	-	0/2/2/2	0/0/0/0
3	DMF	X	16	-	-	0/2/2/2	0/0/0/0
4	SA6	X	300	2	-	0/6/47/47	0/2/2/2
3	DMF	X	40	-	-	0/2/2/2	0/0/0/0
3	DMF	X	41	-	-	0/2/2/2	0/0/0/0
3	DMF	Y	249	-	-	0/2/2/2	0/0/0/0
3	DMF	Y	250	-	-	0/2/2/2	0/0/0/0
3	DMF	Y	251	-	-	0/2/2/2	0/0/0/0
3	DMF	Z	114	-	-	0/2/2/2	0/0/0/0
3	DMF	Z	18	-	-	0/2/2/2	0/0/0/0
4	SA6	Z	300	2	-	0/6/47/47	0/2/2/2
3	DMF	Z	54	-	-	0/2/2/2	0/0/0/0
3	DMF	Z	94	-	-	0/2/2/2	0/0/0/0

All (107) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	R	300	SA6	C7-N9	-4.53	1.29	1.34
4	L	300	SA6	C7-N9	-3.86	1.29	1.34
4	C	300	SA6	C7-N9	-3.37	1.30	1.34
4	Z	300	SA6	C7-N9	-3.11	1.30	1.34
4	H	300	SA6	C7-N9	-2.71	1.31	1.34
4	T	300	SA6	C7-N9	-2.18	1.32	1.34
4	H	300	SA6	O6-C4	2.01	1.47	1.43
4	E	300	SA6	C20-C19	2.03	1.37	1.32
4	2	300	SA6	C15-C20	2.04	1.53	1.50
4	N	300	SA6	C15-C20	2.06	1.53	1.50
4	Z	300	SA6	C3-C7	2.07	1.55	1.52
4	X	300	SA6	C20-C19	2.11	1.38	1.32
4	G	300	SA6	C20-C19	2.13	1.38	1.32
4	N	300	SA6	C3-C7	2.13	1.55	1.52
4	Z	300	SA6	C20-C19	2.15	1.38	1.32
4	L	300	SA6	O6-C4	2.16	1.47	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	Z	300	SA6	O6-C4	2.18	1.47	1.43
4	C	300	SA6	C3-C7	2.19	1.55	1.52
4	R	300	SA6	C15-C20	2.25	1.54	1.50
4	G	300	SA6	O6-C4	2.25	1.47	1.43
4	P	300	SA6	C20-C19	2.30	1.38	1.32
4	X	300	SA6	O14-C13	2.35	1.47	1.42
4	J	300	SA6	C15-C20	2.49	1.54	1.50
4	V	300	SA6	O6-C4	2.50	1.47	1.43
4	J	300	SA6	C20-C19	2.55	1.39	1.32
4	V	300	SA6	C18-C19	2.57	1.57	1.48
4	H	300	SA6	O14-C13	2.61	1.48	1.42
4	N	300	SA6	O14-C13	2.67	1.48	1.42
4	Z	300	SA6	O14-C13	2.75	1.48	1.42
4	J	300	SA6	O6-C4	2.78	1.48	1.43
4	R	300	SA6	O14-C13	2.80	1.48	1.42
4	E	300	SA6	C3-C7	2.90	1.56	1.52
4	L	300	SA6	C15-C20	2.92	1.55	1.50
4	X	300	SA6	O6-C4	2.98	1.48	1.43
4	H	300	SA6	C4-C3	2.98	1.58	1.55
4	T	300	SA6	O6-C4	3.02	1.48	1.43
4	E	300	SA6	O6-C4	3.04	1.48	1.43
4	L	300	SA6	C2-C3	3.08	1.58	1.54
4	J	300	SA6	C2-C3	3.10	1.58	1.54
4	P	300	SA6	C4-C3	3.13	1.58	1.55
4	2	300	SA6	C2-C3	3.18	1.58	1.54
4	Z	300	SA6	C15-C20	3.20	1.55	1.50
4	P	300	SA6	C15-C20	3.28	1.55	1.50
4	T	300	SA6	C15-C20	3.32	1.55	1.50
4	V	300	SA6	O14-C13	3.33	1.49	1.42
4	L	300	SA6	C15-C13	3.35	1.59	1.54
4	G	300	SA6	C15-C20	3.37	1.55	1.50
4	J	300	SA6	O14-C13	3.38	1.49	1.42
4	E	300	SA6	C4-C3	3.38	1.58	1.55
4	T	300	SA6	C2-C3	3.43	1.58	1.54
4	X	300	SA6	C15-C13	3.51	1.60	1.54
4	X	300	SA6	C15-C20	3.56	1.56	1.50
4	Z	300	SA6	C4-C3	3.63	1.59	1.55
4	V	300	SA6	C15-C13	3.72	1.60	1.54
4	Z	300	SA6	C15-C13	3.74	1.60	1.54
4	X	300	SA6	C4-C3	3.77	1.59	1.55
4	N	300	SA6	C15-C13	3.82	1.60	1.54
4	C	300	SA6	C15-C13	3.88	1.60	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	2	300	SA6	C15-C13	3.88	1.60	1.54
4	P	300	SA6	C2-C3	3.99	1.59	1.54
4	V	300	SA6	C15-C20	4.07	1.57	1.50
4	P	300	SA6	C15-C13	4.09	1.61	1.54
4	Z	300	SA6	C2-C3	4.11	1.59	1.54
4	E	300	SA6	C15-C13	4.14	1.61	1.54
4	V	300	SA6	C2-C3	4.16	1.59	1.54
4	E	300	SA6	C2-C3	4.19	1.59	1.54
4	N	300	SA6	C2-C3	4.22	1.59	1.54
4	C	300	SA6	C5-C4	4.50	1.58	1.52
4	G	300	SA6	C2-C3	4.61	1.60	1.54
4	J	300	SA6	C5-C4	4.62	1.58	1.52
4	T	300	SA6	C15-C13	4.63	1.61	1.54
4	H	300	SA6	C15-C13	4.64	1.61	1.54
4	H	300	SA6	C2-C3	4.76	1.60	1.54
4	H	300	SA6	C16-C15	4.80	1.62	1.53
4	R	300	SA6	C15-C13	4.84	1.62	1.54
4	2	300	SA6	C5-C4	4.92	1.58	1.52
4	J	300	SA6	C4-C3	5.04	1.60	1.55
4	G	300	SA6	C15-C13	5.16	1.62	1.54
4	V	300	SA6	C5-C4	5.18	1.59	1.52
4	N	300	SA6	C16-C15	5.22	1.63	1.53
4	E	300	SA6	C5-C4	5.27	1.59	1.52
4	L	300	SA6	C4-C3	5.27	1.60	1.55
4	X	300	SA6	C2-C3	5.31	1.61	1.54
4	E	300	SA6	C16-C15	5.34	1.63	1.53
4	2	300	SA6	C16-C15	5.40	1.63	1.53
4	P	300	SA6	C5-C4	5.56	1.59	1.52
4	X	300	SA6	C16-C15	5.65	1.64	1.53
4	G	300	SA6	C5-C4	5.71	1.59	1.52
4	T	300	SA6	C16-C15	5.80	1.64	1.53
4	P	300	SA6	C16-C15	5.84	1.64	1.53
4	N	300	SA6	C5-C4	5.98	1.60	1.52
4	J	300	SA6	C16-C15	6.01	1.65	1.53
4	C	300	SA6	C2-C3	6.12	1.62	1.54
4	C	300	SA6	C16-C15	6.16	1.65	1.53
4	R	300	SA6	C16-C15	6.18	1.65	1.53
4	X	300	SA6	C5-C4	6.24	1.60	1.52
4	L	300	SA6	C16-C15	6.30	1.65	1.53
4	Z	300	SA6	C16-C15	6.36	1.65	1.53
4	J	300	SA6	C15-C13	6.40	1.64	1.54
4	G	300	SA6	C16-C15	6.46	1.65	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	V	300	SA6	C16-C15	6.63	1.66	1.53
4	L	300	SA6	C5-C4	6.78	1.61	1.52
4	H	300	SA6	C5-C4	6.86	1.61	1.52
4	R	300	SA6	C2-C3	7.01	1.63	1.54
4	Z	300	SA6	C5-C4	7.06	1.61	1.52
4	T	300	SA6	C5-C4	7.42	1.61	1.52
4	R	300	SA6	C5-C4	7.96	1.62	1.52

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	X	300	SA6	C4-C3-C7	-5.22	99.79	104.25
4	T	300	SA6	C4-C3-C7	-5.03	99.95	104.25
4	R	300	SA6	C4-C3-C7	-4.59	100.32	104.25
4	C	300	SA6	C4-C3-C7	-4.57	100.34	104.25
4	P	300	SA6	C4-C3-C7	-4.56	100.35	104.25
4	Z	300	SA6	C4-C3-C7	-4.11	100.73	104.25
4	N	300	SA6	C4-C3-C7	-4.08	100.76	104.25
4	2	300	SA6	C4-C3-C7	-4.03	100.80	104.25
4	V	300	SA6	C4-C3-C7	-3.97	100.85	104.25
4	E	300	SA6	C4-C3-C7	-3.94	100.87	104.25
4	H	300	SA6	C4-C3-C7	-3.89	100.92	104.25
4	J	300	SA6	C4-C3-C7	-3.73	101.06	104.25
4	L	300	SA6	C4-C3-C7	-3.68	101.10	104.25
4	G	300	SA6	C4-C3-C7	-3.34	101.39	104.25
4	L	300	SA6	O14-C13-C15	-3.08	103.04	109.98
4	2	300	SA6	O14-C13-C15	-2.59	104.14	109.98
4	C	300	SA6	O14-C13-C15	-2.55	104.23	109.98
4	T	300	SA6	O14-C13-C15	-2.54	104.25	109.98
4	C	300	SA6	O6-C4-C5	-2.53	102.51	108.39
4	H	300	SA6	O6-C4-C5	-2.38	102.84	108.39
4	P	300	SA6	O8-C7-C3	-2.37	123.52	126.13
4	L	300	SA6	O6-C4-C5	-2.32	102.97	108.39
4	E	300	SA6	O6-C4-C5	-2.22	103.21	108.39
4	P	300	SA6	O6-C4-C5	-2.18	103.31	108.39
4	Z	300	SA6	O6-C4-C5	-2.18	103.32	108.39
4	T	300	SA6	O8-C7-C3	-2.13	123.78	126.13
4	2	300	SA6	O8-C7-C3	-2.12	123.79	126.13
4	V	300	SA6	O8-C7-C3	-2.12	123.80	126.13
4	H	300	SA6	O14-C13-C15	-2.11	105.22	109.98
4	R	300	SA6	O14-C13-C15	-2.11	105.22	109.98
4	J	300	SA6	O8-C7-C3	-2.07	123.85	126.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	2	300	SA6	O6-C4-C5	-2.03	103.65	108.39
4	N	300	SA6	C16-C15-C13	2.02	118.24	113.36
4	L	300	SA6	C1-C2-C3	2.03	119.99	114.19
4	N	300	SA6	C10-C13-C15	2.04	116.65	114.09
4	C	300	SA6	C17-C16-C15	2.08	115.19	111.50
4	R	300	SA6	C17-C16-C15	2.13	115.29	111.50
4	J	300	SA6	C17-C16-C15	2.15	115.31	111.50
4	H	300	SA6	C17-C16-C15	2.18	115.37	111.50
4	R	300	SA6	C16-C15-C13	2.23	118.75	113.36
4	N	300	SA6	C1-C2-C3	2.23	120.56	114.19
4	E	300	SA6	C1-C2-C3	2.30	120.78	114.19
4	Z	300	SA6	C17-C16-C15	2.34	115.65	111.50
4	E	300	SA6	C2-C3-C4	2.35	119.20	115.53
4	V	300	SA6	C17-C16-C15	2.39	115.75	111.50
4	2	300	SA6	C17-C16-C15	2.40	115.75	111.50
4	J	300	SA6	C10-C13-C15	2.44	117.15	114.09
4	C	300	SA6	C2-C3-C4	2.52	119.46	115.53
4	H	300	SA6	C10-C13-C15	2.54	117.28	114.09
4	R	300	SA6	C10-C13-C15	2.60	117.35	114.09
4	G	300	SA6	C10-C13-C15	2.79	117.59	114.09
4	2	300	SA6	C2-C3-C4	2.81	119.92	115.53
4	P	300	SA6	C10-C13-C15	2.86	117.68	114.09
4	N	300	SA6	C2-C3-C4	2.90	120.06	115.53
4	L	300	SA6	C2-C3-C4	2.94	120.12	115.53
4	C	300	SA6	C10-C13-C15	3.22	118.13	114.09
4	2	300	SA6	C10-C13-C15	3.42	118.39	114.09
4	E	300	SA6	C10-C13-C15	3.59	118.60	114.09
4	T	300	SA6	C10-C13-C15	3.71	118.75	114.09
4	L	300	SA6	C10-C13-C15	4.01	119.12	114.09

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

105 monomers are involved in 314 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	2	101	DMF	2	0
3	2	108	DMF	5	0
3	2	112	DMF	7	0
4	2	300	SA6	4	0
3	2	4	DMF	8	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	2	49	DMF	1	0
3	2	52	DMF	2	0
3	2	87	DMF	2	0
3	A	249	DMF	1	0
3	B	249	DMF	2	0
3	C	103	DMF	8	0
4	C	300	SA6	3	0
3	C	38	DMF	3	0
3	C	47	DMF	1	0
3	C	63	DMF	1	0
3	C	69	DMF	1	0
3	C	88	DMF	1	0
3	D	251	DMF	4	0
3	D	253	DMF	2	0
3	E	100	DMF	2	0
3	E	20	DMF	4	0
3	E	28	DMF	1	0
4	E	300	SA6	3	0
3	E	53	DMF	2	0
3	E	73	DMF	3	0
3	E	75	DMF	4	0
3	F	250	DMF	1	0
3	G	111	DMF	1	0
3	G	119	DMF	11	0
3	G	12	DMF	4	0
3	G	24	DMF	2	0
4	G	300	SA6	3	0
3	G	62	DMF	1	0
3	G	64	DMF	9	0
3	G	70	DMF	1	0
3	G	98	DMF	2	0
3	H	117	DMF	2	0
4	H	300	SA6	5	0
3	H	43	DMF	4	0
3	H	66	DMF	3	0
3	H	71	DMF	1	0
3	H	91	DMF	2	0
3	I	250	DMF	2	0
3	J	123	DMF	6	0
4	J	300	SA6	2	0
3	J	45	DMF	1	0
3	K	249	DMF	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	K	250	DMF	4	0
3	K	251	DMF	3	0
3	K	252	DMF	3	0
4	L	300	SA6	3	0
3	L	81	DMF	1	0
3	L	97	DMF	4	0
3	N	104	DMF	7	0
3	N	118	DMF	4	0
3	N	22	DMF	4	0
4	N	300	SA6	3	0
3	N	90	DMF	7	0
3	N	93	DMF	4	0
3	O	250	DMF	1	0
3	P	107	DMF	5	0
3	P	14	DMF	5	0
3	P	2	DMF	1	0
4	P	300	SA6	4	0
3	P	33	DMF	3	0
3	Q	249	DMF	2	0
3	Q	250	DMF	6	0
3	Q	251	DMF	1	0
4	R	300	SA6	3	0
3	R	59	DMF	9	0
3	R	80	DMF	1	0
3	R	92	DMF	2	0
3	R	95	DMF	1	0
3	S	249	DMF	1	0
3	T	102	DMF	3	0
3	T	113	DMF	5	0
3	T	115	DMF	1	0
3	T	29	DMF	3	0
4	T	300	SA6	3	0
3	T	84	DMF	3	0
3	U	250	DMF	8	0
3	V	116	DMF	6	0
3	V	120	DMF	8	0
3	V	27	DMF	8	0
4	V	300	SA6	4	0
3	V	32	DMF	5	0
3	V	39	DMF	1	0
3	V	42	DMF	7	0
3	V	82	DMF	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	V	83	DMF	11	0
3	W	249	DMF	2	0
3	W	250	DMF	5	0
3	X	122	DMF	1	0
3	X	15	DMF	1	0
3	X	16	DMF	3	0
4	X	300	SA6	4	0
3	X	40	DMF	1	0
3	X	41	DMF	1	0
3	Y	249	DMF	1	0
3	Y	250	DMF	1	0
3	Y	251	DMF	2	0
3	Z	18	DMF	2	0
4	Z	300	SA6	3	0
3	Z	54	DMF	3	0
3	Z	94	DMF	3	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<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	1	215/248 (86%)	0.40	17 (7%) 13 12	19, 48, 88, 109	0
1	A	215/248 (86%)	0.68	30 (13%) 3 3	20, 54, 91, 107	0
1	B	213/248 (85%)	0.46	15 (7%) 17 16	20, 49, 88, 106	0
1	D	214/248 (86%)	1.25	59 (27%) 1 0	20, 65, 98, 110	0
1	F	220/248 (88%)	0.47	17 (7%) 14 13	17, 48, 86, 104	0
1	I	216/248 (87%)	0.57	28 (12%) 4 3	18, 52, 92, 108	0
1	K	216/248 (87%)	0.53	19 (8%) 11 9	21, 55, 92, 107	0
1	M	216/248 (87%)	0.70	32 (14%) 3 2	18, 53, 92, 104	0
1	O	216/248 (87%)	0.57	24 (11%) 6 5	17, 49, 87, 102	0
1	Q	215/248 (86%)	0.49	20 (9%) 9 8	22, 50, 86, 99	0
1	S	216/248 (87%)	0.71	32 (14%) 3 2	20, 56, 91, 104	0
1	U	216/248 (87%)	0.47	25 (11%) 5 5	16, 49, 86, 102	0
1	W	216/248 (87%)	0.97	43 (19%) 1 1	20, 63, 94, 107	0
1	Y	216/248 (87%)	0.80	31 (14%) 3 2	22, 58, 94, 123	0
2	2	223/240 (92%)	-0.47	1 (0%) 92 91	11, 21, 45, 65	0
2	C	222/240 (92%)	-0.51	2 (0%) 84 83	8, 20, 48, 79	0
2	E	223/240 (92%)	-0.49	2 (0%) 84 83	8, 20, 46, 63	0
2	G	222/240 (92%)	-0.47	1 (0%) 90 90	10, 23, 53, 75	0
2	H	222/240 (92%)	-0.50	0 100 100	9, 23, 50, 71	0
2	J	222/240 (92%)	-0.48	1 (0%) 90 90	9, 21, 49, 70	0
2	L	223/240 (92%)	-0.45	1 (0%) 92 91	8, 21, 46, 66	0
2	N	222/240 (92%)	-0.48	1 (0%) 90 90	8, 21, 47, 79	0
2	P	222/240 (92%)	-0.50	0 100 100	10, 23, 49, 73	0
2	R	239/240 (99%)	-0.50	4 (1%) 70 68	8, 20, 55, 83	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å <sup>2</sup> )	Q<0.9
2	T	223/240 (92%)	-0.39	1 (0%)	92 91	10, 24, 53, 72	0
2	V	239/240 (99%)	-0.48	3 (1%)	77 75	8, 20, 63, 91	0
2	X	223/240 (92%)	-0.46	3 (1%)	77 75	10, 24, 56, 73	0
2	Z	223/240 (92%)	-0.43	3 (1%)	77 75	11, 24, 52, 69	0
All	All	6168/6832 (90%)	0.08	415 (6%)	19 17	8, 33, 84, 123	0

All (415) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	6	PHE	8.4
1	M	203	LEU	7.5
1	S	7	ILE	7.0
1	I	203	LEU	6.9
1	Y	8	SER	6.8
1	A	191	GLY	6.7
1	I	7	ILE	6.5
1	D	159	THR	6.4
1	Q	7	ILE	6.4
1	F	6	PHE	6.2
1	Y	203	LEU	5.9
1	O	203	LEU	5.8
1	Y	9	PRO	5.7
1	D	233	LEU	5.6
1	B	7	ILE	5.5
1	W	233	LEU	5.4
1	U	204	GLY	5.3
1	M	172	ALA	5.3
1	K	7	ILE	5.3
1	W	172	ALA	5.2
1	O	7	ILE	5.1
1	F	5	TYR	5.0
1	O	172	ALA	5.0
2	2	523	GLY	4.9
1	D	205	VAL	4.8
1	O	206	ALA	4.7
1	1	203	LEU	4.7
1	F	192	SER	4.7
2	X	523	GLY	4.7
1	W	162	PRO	4.6
1	D	169	GLU	4.6
1	K	203	LEU	4.6

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Mol	Chain	Res	Type	RSRZ
1	S	162	PRO	4.5
1	W	46	PRO	4.4
1	S	235	VAL	4.4
1	D	172	ALA	4.3
1	D	234	LEU	4.3
1	S	8	SER	4.3
1	D	206	ALA	4.2
1	W	189	ARG	4.2
1	D	226	THR	4.2
1	D	204	GLY	4.2
1	D	231	GLN	4.2
1	D	160	THR	4.2
1	K	11	GLN	4.1
1	W	182	ARG	4.1
1	D	161	GLU	4.1
1	D	8	SER	4.1
1	1	8	SER	4.1
1	W	163	ILE	4.1
1	K	228	SER	4.1
1	W	228	SER	4.0
1	U	7	ILE	4.0
1	S	41	PHE	3.9
1	D	171	TYR	3.9
1	M	12	ALA	3.9
1	D	179	ASP	3.9
1	S	204	GLY	3.8
1	A	205	VAL	3.8
1	S	161	GLU	3.8
1	W	232	ALA	3.8
1	K	204	GLY	3.7
1	F	7	ILE	3.7
1	Y	7	ILE	3.7
1	Y	31	VAL	3.7
2	L	523	GLY	3.7
1	U	205	VAL	3.7
1	B	49	SER	3.7
1	W	204	GLY	3.7
1	A	172	ALA	3.7
1	U	171	TYR	3.7
1	M	8	SER	3.6
1	D	42	VAL	3.6
1	A	189	ARG	3.6

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Mol	Chain	Res	Type	RSRZ
1	M	167	LEU	3.6
1	D	48	ARG	3.6
1	K	10	GLU	3.6
1	M	205	VAL	3.6
1	D	36	ALA	3.6
1	D	46	PRO	3.6
1	F	169	GLU	3.6
1	U	173	GLU	3.5
1	O	189	ARG	3.5
1	D	207	SER	3.5
2	E	523	GLY	3.5
1	Y	30	VAL	3.5
1	B	171	TYR	3.5
1	D	131	GLY	3.5
1	S	207	SER	3.5
1	W	131	GLY	3.5
1	M	133	THR	3.5
2	V	530	ASP	3.4
1	M	25	ALA	3.4
1	Y	10	GLU	3.4
1	M	227	GLY	3.4
1	S	159	THR	3.4
1	U	206	ALA	3.4
1	S	171	TYR	3.4
1	D	228	SER	3.3
1	D	165	ASN	3.3
1	K	232	ALA	3.3
1	F	133	THR	3.3
1	A	188	LEU	3.3
1	D	167	LEU	3.3
1	D	41	PHE	3.3
1	K	189	ARG	3.3
1	W	48	ARG	3.3
1	O	173	GLU	3.3
1	U	8	SER	3.3
1	A	48	ARG	3.3
1	1	206	ALA	3.3
1	A	135	ARG	3.3
1	Q	8	SER	3.2
1	U	233	LEU	3.2
2	Z	523	GLY	3.2
2	R	530	ASP	3.2

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Mol	Chain	Res	Type	RSRZ
1	M	31	VAL	3.2
1	D	158	GLY	3.2
1	Q	131	GLY	3.2
1	D	180	ALA	3.2
1	A	46	PRO	3.2
1	Y	11	GLN	3.2
1	D	25	ALA	3.2
1	K	206	ALA	3.2
1	D	189	ARG	3.1
1	W	122	LEU	3.1
1	W	231	GLN	3.1
1	F	170	SER	3.1
1	D	182	ARG	3.1
1	O	48	ARG	3.1
1	I	41	PHE	3.1
1	D	227	GLY	3.1
1	S	169	GLU	3.1
1	B	231	GLN	3.1
1	D	40	LEU	3.1
1	A	163	ILE	3.1
1	O	205	VAL	3.0
1	Q	204	GLY	3.0
1	I	63	ALA	3.0
1	Y	41	PHE	3.0
1	D	188	LEU	3.0
1	W	206	ALA	3.0
1	Y	26	ARG	3.0
1	W	28	LYS	3.0
1	A	161	GLU	3.0
1	Q	113	GLU	3.0
1	W	135	ARG	3.0
2	R	539	HIS	3.0
1	D	133	THR	3.0
1	A	167	LEU	2.9
1	A	131	GLY	2.9
1	I	8	SER	2.9
1	S	229	ALA	2.9
1	1	168	LYS	2.9
1	A	190	ALA	2.9
1	M	48	ARG	2.9
1	M	46	PRO	2.9
2	G	412	SER	2.9

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Mol	Chain	Res	Type	RSRZ
1	S	158	GLY	2.9
1	A	206	ALA	2.9
1	A	169	GLU	2.9
1	A	226	THR	2.9
1	M	49	SER	2.9
1	A	207	SER	2.9
1	W	234	LEU	2.9
1	D	47	SER	2.8
2	N	412	SER	2.8
1	M	180	ALA	2.8
1	Y	172	ALA	2.8
1	F	41	PHE	2.8
1	K	131	GLY	2.8
1	U	131	GLY	2.8
1	Y	131	GLY	2.8
1	D	21	ARG	2.8
1	D	229	ALA	2.8
1	S	172	ALA	2.8
1	S	188	LEU	2.8
1	M	169	GLU	2.8
1	W	31	VAL	2.8
1	Y	229	ALA	2.8
1	M	189	ARG	2.8
1	Y	63	ALA	2.8
1	A	227	GLY	2.8
1	M	228	SER	2.8
1	1	159	THR	2.8
1	D	10	GLU	2.8
1	1	48	ARG	2.8
1	F	25	ALA	2.7
1	Y	12	ALA	2.7
1	D	14	ARG	2.7
1	K	205	VAL	2.7
1	O	39	VAL	2.7
1	U	169	GLU	2.7
1	O	14	ARG	2.7
1	S	133	THR	2.7
1	A	11	GLN	2.7
1	I	158	GLY	2.7
1	S	163	ILE	2.7
2	C	412	SER	2.7
1	Y	135	ARG	2.7

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Mol	Chain	Res	Type	RSRZ
1	I	135	ARG	2.7
1	Y	14	ARG	2.7
1	D	163	ILE	2.7
1	I	12	ALA	2.7
1	I	11	GLN	2.7
1	I	188	LEU	2.7
1	W	40	LEU	2.7
1	W	158	GLY	2.7
1	W	165	ASN	2.6
1	I	190	ALA	2.6
1	Q	172	ALA	2.6
1	O	41	PHE	2.6
1	U	133	THR	2.6
1	A	204	GLY	2.6
1	W	167	LEU	2.6
1	D	162	PRO	2.6
1	K	229	ALA	2.6
1	F	48	ARG	2.6
1	I	31	VAL	2.6
1	I	205	VAL	2.6
1	1	179	ASP	2.6
1	F	172	ALA	2.6
1	W	7	ILE	2.6
1	F	191	GLY	2.6
1	K	227	GLY	2.6
1	M	204	GLY	2.6
1	W	171	TYR	2.6
1	B	173	GLU	2.6
1	M	131	GLY	2.6
1	W	227	GLY	2.6
1	1	41	PHE	2.6
1	O	135	ARG	2.6
1	K	48	ARG	2.6
1	I	171	TYR	2.6
1	M	231	GLN	2.6
1	O	231	GLN	2.6
1	U	161	GLU	2.6
1	A	228	SER	2.5
1	W	161	GLU	2.5
1	U	232	ALA	2.5
1	D	135	ARG	2.5
1	M	7	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
1	O	10	GLU	2.5
1	D	185	VAL	2.5
2	C	416	SER	2.5
1	O	161	GLU	2.5
1	W	179	ASP	2.5
1	Q	205	VAL	2.5
1	B	206	ALA	2.5
1	M	173	GLU	2.5
2	T	412	SER	2.5
1	A	133	THR	2.5
1	I	189	ARG	2.5
1	Q	48	ARG	2.5
1	U	48	ARG	2.5
2	V	535	HIS	2.5
1	D	177	LEU	2.5
1	B	161	GLU	2.5
1	Y	169	GLU	2.5
1	A	171	TYR	2.5
1	W	26	ARG	2.5
1	S	167	LEU	2.5
1	W	205	VAL	2.5
1	A	180	ALA	2.5
1	O	25	ALA	2.5
1	B	182	ARG	2.5
1	B	165	ASN	2.5
1	1	163	ILE	2.5
1	U	11	GLN	2.5
1	K	8	SER	2.4
1	M	9	PRO	2.4
2	R	412	SER	2.4
1	D	151	PRO	2.4
1	S	12	ALA	2.4
1	D	30	VAL	2.4
1	Y	42	VAL	2.4
1	1	11	GLN	2.4
1	Q	182	ARG	2.4
1	D	130	TYR	2.4
1	D	11	GLN	2.4
1	O	40	LEU	2.4
1	Q	169	GLU	2.4
1	Y	226	THR	2.4
1	A	165	ASN	2.4

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Mol	Chain	Res	Type	RSRZ
1	S	40	LEU	2.4
1	B	191	GLY	2.4
1	D	32	ALA	2.4
1	I	206	ALA	2.4
1	1	172	ALA	2.4
1	W	178	THR	2.4
1	D	18	GLU	2.4
1	W	44	GLU	2.4
1	D	183	ILE	2.4
1	F	135	ARG	2.4
1	I	14	ARG	2.4
1	I	182	ARG	2.4
1	S	227	GLY	2.4
1	A	234	LEU	2.4
1	1	40	LEU	2.4
1	D	170	SER	2.4
1	A	182	ARG	2.3
1	K	233	LEU	2.3
1	M	175	ALA	2.3
1	Y	123	CYS	2.3
1	I	131	GLY	2.3
1	Q	173	GLU	2.3
1	1	15	GLU	2.3
2	R	535	HIS	2.3
1	S	206	ALA	2.3
1	I	48	ARG	2.3
1	W	159	THR	2.3
1	B	170	SER	2.3
1	K	170	SER	2.3
1	O	8	SER	2.3
1	S	228	SER	2.3
1	F	205	VAL	2.3
1	A	44	GLU	2.3
1	D	157	GLY	2.3
1	W	49	SER	2.3
1	F	14	ARG	2.3
1	Q	41	PHE	2.3
1	W	18	GLU	2.3
1	I	125	ALA	2.3
1	M	206	ALA	2.3
1	M	171	TYR	2.3
1	F	227	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	U	26	ARG	2.3
2	J	415	GLN	2.3
1	S	165	ASN	2.2
1	O	31	VAL	2.2
1	D	232	ALA	2.2
1	U	25	ALA	2.2
1	Y	175	ALA	2.2
1	O	226	THR	2.2
1	W	133	THR	2.2
1	Y	189	ARG	2.2
1	W	208	LEU	2.2
2	Z	414	PRO	2.2
1	B	189	ARG	2.2
1	U	228	SER	2.2
1	D	168	LYS	2.2
1	O	204	GLY	2.2
1	D	152	HIS	2.2
2	X	396	GLN	2.2
1	S	135	ARG	2.2
1	S	205	VAL	2.2
1	K	133	THR	2.2
1	D	230	LEU	2.2
1	U	182	ARG	2.2
1	I	30	VAL	2.2
1	O	169	GLU	2.2
2	Z	415	GLN	2.2
1	Q	133	THR	2.2
1	W	180	ALA	2.2
1	S	26	ARG	2.2
1	S	189	ARG	2.2
1	1	10	GLU	2.2
1	M	11	GLN	2.2
1	U	191	GLY	2.2
1	K	26	ARG	2.1
1	W	41	PHE	2.1
1	Y	44	GLU	2.1
1	1	161	GLU	2.1
2	E	412	SER	2.1
1	I	169	GLU	2.1
1	S	42	VAL	2.1
1	Q	63	ALA	2.1
1	S	63	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	U	163	ILE	2.1
1	I	165	ASN	2.1
1	D	26	ARG	2.1
1	S	123	CYS	2.1
1	S	182	ARG	2.1
1	U	44	GLU	2.1
1	W	169	GLU	2.1
1	Q	159	THR	2.1
1	B	207	SER	2.1
1	M	10	GLU	2.1
1	Y	161	GLU	2.1
1	Y	227	GLY	2.1
1	I	42	VAL	2.1
1	Q	130	TYR	2.1
2	V	533	GLU	2.1
1	A	231	GLN	2.1
1	W	14	ARG	2.1
1	A	49	SER	2.1
1	B	130	TYR	2.1
1	Q	158	GLY	2.1
1	U	41	PHE	2.1
1	I	161	GLU	2.1
1	F	189	ARG	2.1
1	I	135	ARG	2.1
1	O	133	THR	2.1
1	O	159	THR	2.1
1	Q	174	ASN	2.1
1	W	160	THR	2.1
1	M	226	THR	2.0
1	Q	228	SER	2.0
1	M	42	VAL	2.0
1	U	46	PRO	2.0
1	W	130	TYR	2.0
1	M	163	ILE	2.0
1	Y	163	ILE	2.0
1	B	13	MET	2.0
1	Y	150	GLU	2.0
1	Y	228	SER	2.0
1	Y	165	ASN	2.0
1	Y	171	TYR	2.0
1	I	227	GLY	2.0
2	X	397	GLY	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	49	SER	2.0
1	I	232	ALA	2.0
1	M	22	LYS	2.0
1	Q	26	ARG	2.0
1	U	189	ARG	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	DMF	P	2	5/5	0.82	0.31	35.44	62,62,64,64	0
3	DMF	N	118	5/5	0.92	0.37	27.20	20,20,20,20	0
3	DMF	G	24	5/5	0.80	0.40	25.36	65,67,68,68	0
3	DMF	T	84	5/5	0.68	0.45	25.34	59,59,60,62	0
3	DMF	C	63	5/5	0.80	0.23	21.50	58,59,59,60	0
3	DMF	V	27	5/5	0.87	0.32	20.52	63,63,64,64	0
3	DMF	E	20	5/5	0.84	0.44	20.44	76,77,77,78	0
3	DMF	G	111	5/5	0.86	0.40	20.15	20,20,20,20	0
3	DMF	D	252	5/5	0.86	0.33	17.30	20,20,20,20	0
3	DMF	N	93	5/5	0.88	0.32	17.16	20,20,20,20	0
3	DMF	2	87	5/5	0.96	0.37	16.59	20,20,20,20	0
3	DMF	L	81	5/5	0.61	0.51	16.24	59,60,61,62	0
3	DMF	V	120	5/5	0.84	0.39	15.58	20,20,20,20	0
3	DMF	T	102	5/5	0.80	0.43	15.45	20,20,20,20	0
3	DMF	R	59	5/5	0.77	0.43	14.81	54,55,57,57	0
3	DMF	2	108	5/5	0.83	0.45	14.76	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	DMF	2	112	5/5	0.79	0.48	14.41	20,20,20,20	0
3	DMF	Z	18	5/5	0.80	0.28	14.41	55,55,55,55	0
3	DMF	D	253	5/5	0.52	0.45	14.21	20,20,20,20	0
3	DMF	C	88	5/5	0.88	0.43	14.12	20,20,20,20	0
3	DMF	Z	114	5/5	0.80	0.45	14.09	20,20,20,20	0
3	DMF	H	117	5/5	0.76	0.42	13.64	20,20,20,20	0
3	DMF	V	82	5/5	0.78	0.36	13.62	45,47,47,48	0
3	DMF	F	249	5/5	0.64	0.43	13.62	90,91,91,91	0
3	DMF	Z	94	5/5	0.87	0.45	13.61	20,20,20,20	0
3	DMF	V	109	5/5	0.85	0.42	13.37	20,20,20,20	0
3	DMF	X	122	5/5	0.65	0.33	13.18	20,20,20,20	0
3	DMF	R	95	5/5	0.77	0.43	13.15	20,20,20,20	0
3	DMF	R	89	5/5	0.85	0.39	13.13	20,20,20,20	0
3	DMF	M	252	5/5	0.89	0.29	13.12	20,20,20,20	0
3	DMF	C	103	5/5	0.82	0.42	13.07	20,20,20,20	0
3	DMF	T	113	5/5	0.86	0.48	13.06	20,20,20,20	0
3	DMF	J	123	5/5	0.87	0.53	13.01	20,20,20,20	0
3	DMF	G	64	5/5	0.79	0.40	12.93	66,68,68,69	0
3	DMF	G	119	5/5	0.85	0.44	12.72	20,20,20,20	0
3	DMF	V	42	5/5	0.90	0.27	12.71	58,58,59,61	0
3	DMF	J	110	5/5	0.84	0.44	12.44	20,20,20,20	0
3	DMF	N	104	5/5	0.74	0.48	12.22	20,20,20,20	0
3	DMF	N	90	5/5	0.93	0.32	12.13	20,20,20,20	0
3	DMF	G	70	5/5	0.81	0.28	12.06	37,38,41,41	0
3	DMF	P	107	5/5	0.89	0.34	12.02	20,20,20,20	0
3	DMF	O	249	5/5	0.89	0.19	11.89	39,40,41,41	0
3	DMF	E	28	5/5	0.58	0.34	11.58	61,61,63,64	0
3	DMF	T	115	5/5	0.92	0.39	11.57	20,20,20,20	0
3	DMF	C	47	5/5	0.82	0.26	11.40	61,62,62,62	0
3	DMF	G	98	5/5	0.88	0.45	11.38	20,20,20,20	0
3	DMF	J	45	5/5	0.52	0.43	11.11	41,43,45,46	0
3	DMF	2	57	5/5	0.71	0.34	11.07	54,56,57,57	0
3	DMF	A	250	5/5	0.85	0.27	10.98	39,41,42,44	0
3	DMF	Y	249	5/5	0.93	0.22	10.83	62,64,64,65	0
3	DMF	P	14	5/5	0.86	0.28	10.78	56,58,58,59	0
3	DMF	2	52	5/5	0.74	0.27	10.68	77,77,78,78	0
3	DMF	2	49	5/5	0.76	0.33	10.29	57,57,57,58	0
3	DMF	Y	251	5/5	0.84	0.53	9.94	20,20,20,20	0
3	DMF	O	251	5/5	0.73	0.35	9.60	20,20,20,20	0
3	DMF	V	39	5/5	0.74	0.29	9.10	60,60,61,61	0
3	DMF	H	43	5/5	0.90	0.27	8.99	82,82,83,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	DMF	B	250	5/5	0.76	0.30	8.98	53,53,55,55	0
3	DMF	H	72	5/5	0.86	0.44	8.93	20,20,20,20	0
3	DMF	X	41	5/5	0.81	0.26	8.71	61,61,62,62	0
3	DMF	K	250	5/5	0.85	0.33	8.29	77,78,79,79	0
3	DMF	F	251	5/5	0.82	0.26	8.06	54,54,55,55	0
3	DMF	M	251	5/5	0.55	0.34	8.04	64,64,66,66	0
3	DMF	X	16	5/5	0.83	0.22	7.93	86,86,86,86	0
3	DMF	2	101	5/5	0.87	0.38	7.76	20,20,20,20	0
3	DMF	K	251	5/5	0.71	0.37	7.52	63,63,64,64	0
3	DMF	G	77	5/5	0.87	0.24	7.32	49,50,50,51	0
3	DMF	W	250	5/5	0.91	0.22	7.22	63,63,64,64	0
3	DMF	G	12	5/5	0.88	0.33	7.20	60,61,62,63	0
3	DMF	Z	54	5/5	0.75	0.24	7.12	58,59,60,61	0
3	DMF	G	62	5/5	0.75	0.29	6.93	72,73,73,74	0
3	DMF	A	249	5/5	0.84	0.27	6.88	44,44,44,44	0
3	DMF	L	97	5/5	0.91	0.28	6.82	20,20,20,20	0
3	DMF	P	56	5/5	0.92	0.19	6.77	59,60,60,61	0
3	DMF	2	4	5/5	0.88	0.22	6.73	62,62,62,62	0
3	DMF	L	36	5/5	0.84	0.21	6.52	41,42,43,43	0
3	DMF	E	53	5/5	0.77	0.25	6.10	56,57,58,59	0
3	DMF	I	250	5/5	0.92	0.22	6.09	41,41,42,42	0
3	DMF	P	60	5/5	0.81	0.24	5.88	68,69,69,69	0
3	DMF	D	249	5/5	0.86	0.24	5.83	53,53,53,54	0
3	DMF	O	250	5/5	0.87	0.21	5.75	44,45,46,48	0
3	DMF	F	250	5/5	0.86	0.24	5.67	56,56,58,59	0
3	DMF	T	10	5/5	0.80	0.33	5.47	71,72,72,74	0
3	DMF	T	29	5/5	0.88	0.22	5.36	76,76,76,76	0
3	DMF	S	250	5/5	0.81	0.19	5.10	59,59,60,61	0
3	DMF	D	251	5/5	0.86	0.27	5.07	94,95,96,96	0
3	DMF	M	250	5/5	0.78	0.26	5.05	60,61,61,62	0
3	DMF	U	249	5/5	0.83	0.24	5.03	40,40,44,45	0
3	DMF	B	249	5/5	0.88	0.21	5.01	50,51,51,53	0
3	DMF	S	249	5/5	0.91	0.25	4.88	54,54,55,56	0
3	DMF	Q	249	5/5	0.92	0.22	4.82	48,48,49,49	0
3	DMF	W	249	5/5	0.83	0.25	4.61	69,70,71,72	0
3	DMF	V	83	5/5	0.88	0.22	4.57	58,59,60,62	0
3	DMF	V	32	5/5	0.93	0.18	4.39	73,74,74,74	0
3	DMF	U	250	5/5	0.88	0.21	4.22	49,50,51,51	0
3	DMF	E	75	5/5	0.89	0.23	3.82	64,64,64,65	0
3	DMF	K	249	5/5	0.80	0.21	3.78	49,50,51,52	0
3	DMF	X	15	5/5	0.85	0.23	3.73	66,67,68,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	DMF	Y	250	5/5	0.88	0.20	3.55	42,42,44,44	0
3	DMF	M	249	5/5	0.84	0.18	3.50	46,47,48,48	0
3	DMF	D	250	5/5	0.87	0.21	3.12	61,63,64,65	0
3	DMF	Q	250	5/5	0.84	0.28	3.06	84,85,85,86	0
3	DMF	Q	251	5/5	0.91	0.19	2.67	53,53,56,57	0
3	DMF	1	249	5/5	0.91	0.14	2.66	45,47,48,49	0
3	DMF	I	249	5/5	0.93	0.18	2.45	40,42,42,43	0
3	DMF	R	92	5/5	0.94	0.33	1.56	20,20,20,20	0
3	DMF	L	50	5/5	0.82	0.20	1.14	55,56,57,57	0
4	SA6	L	300	20/20	0.93	0.10	0.60	16,19,26,27	0
4	SA6	H	300	20/20	0.92	0.11	0.56	16,21,23,24	0
3	DMF	R	80	5/5	0.88	0.19	0.48	74,75,76,76	0
4	SA6	R	300	20/20	0.95	0.10	0.44	12,21,24,31	0
4	SA6	C	300	20/20	0.96	0.10	0.30	16,19,24,24	0
4	SA6	Z	300	20/20	0.94	0.10	0.26	17,19,22,25	0
4	SA6	V	300	20/20	0.94	0.10	0.24	15,17,21,22	0
4	SA6	N	300	20/20	0.94	0.10	0.22	13,18,23,26	0
4	SA6	2	300	20/20	0.95	0.11	0.19	17,20,28,29	0
4	SA6	P	300	20/20	0.96	0.09	0.12	16,20,28,29	0
4	SA6	J	300	20/20	0.96	0.08	0.04	12,19,24,27	0
4	SA6	E	300	20/20	0.95	0.09	-0.02	12,18,21,24	0
4	SA6	X	300	20/20	0.96	0.09	-0.14	15,17,23,25	0
4	SA6	T	300	20/20	0.94	0.10	-0.17	17,22,28,29	0
4	SA6	G	300	20/20	0.94	0.09	-0.20	11,19,22,24	0
3	DMF	P	33	5/5	0.82	0.20	-	65,66,66,66	0
3	DMF	H	71	5/5	0.91	0.28	-	54,55,55,56	0
3	DMF	E	100	5/5	0.88	0.46	-	20,20,20,20	0
3	DMF	V	116	5/5	0.92	0.21	-	20,20,20,20	0
3	DMF	E	73	5/5	0.64	0.52	-	120,120,121,121	0
3	DMF	C	69	5/5	0.92	0.25	-	48,48,50,50	0
3	DMF	K	252	5/5	0.78	0.37	-	80,81,82,82	0
3	DMF	H	66	5/5	0.80	0.31	-	69,69,69,70	0
3	DMF	P	86	5/5	0.83	0.50	-	20,20,20,20	0
3	DMF	C	121	5/5	0.88	0.24	-	20,20,20,20	0
3	DMF	H	91	5/5	0.86	0.31	-	20,20,20,20	0
3	DMF	N	22	5/5	0.88	0.29	-	44,45,49,50	0
3	DMF	P	51	5/5	0.81	0.23	-	75,76,76,77	0
3	DMF	X	40	5/5	0.73	0.29	-	84,85,85,85	0
3	DMF	C	38	5/5	0.92	0.24	-	64,64,65,65	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.