



Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 09:34 pm BST

PDB ID : 3HFA
Title : Crystal Structure of Mycobacterium Tuberculosis Proteasome open-gate mutant
Authors : Li, D.; Li, H.
Deposited on : 2009-05-11
Resolution : 2.50 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

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

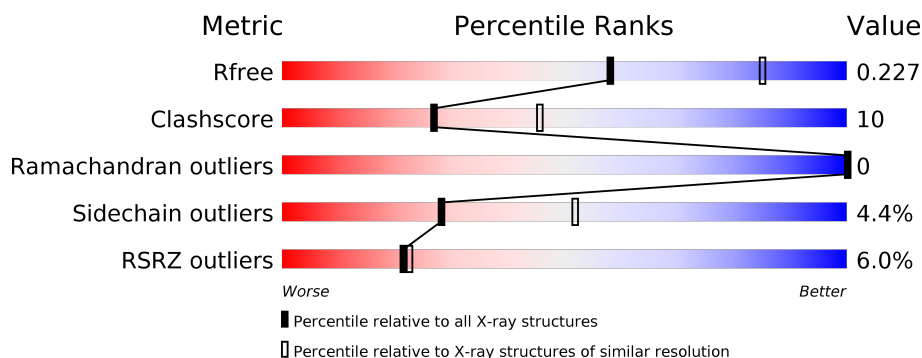
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 Å.

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



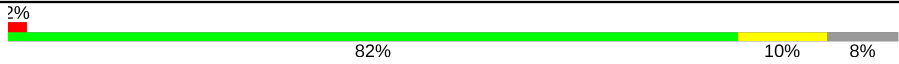




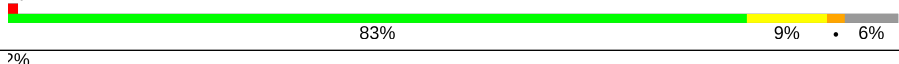


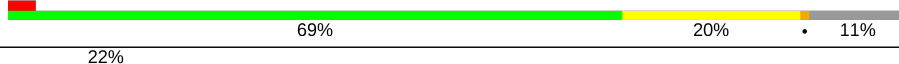
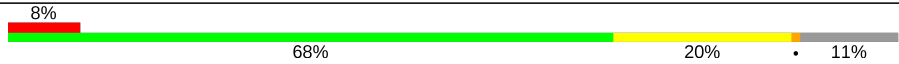

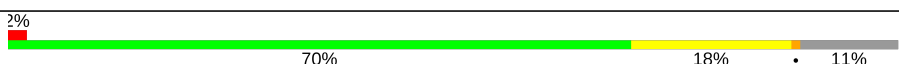
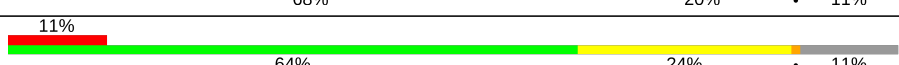








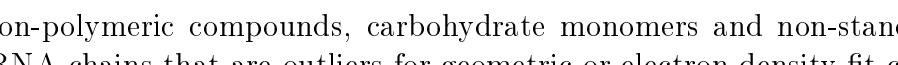
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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

Mol	Chain	Length	Quality of chain
1	2	240	<div> <div>83%</div> <div>9%</div> <div>8%</div> </div>
1	C	240	<div>5%</div> <div>82%</div> <div>10%</div> <div>8%</div>

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Mol	Chain	Length	Quality of chain
1	L	240	
1	N	240	
1	P	240	
1	R	240	
1	T	240	
1	V	240	
1	X	240	
1	Z	240	
2	1	240	
2	A	240	
2	B	240	
2	D	240	
2	F	240	
2	I	240	
2	K	240	
2	M	240	
2	O	240	
2	Q	240	
2	S	240	
2	U	240	
2	W	240	
2	Y	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	K	251	-	-	X	-
3	DMF	Q	251	-	-	X	-
3	DMF	Z	69	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 48523 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 (Beta subunit) PrcB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	223	Total	C	N	O	S	0	0	0
			1642	1029	283	325	5			
1	C	222	Total	C	N	O	S	0	0	0
			1638	1027	282	324	5			
1	E	223	Total	C	N	O	S	0	0	0
			1642	1029	283	325	5			
1	G	222	Total	C	N	O	S	0	0	0
			1638	1027	282	324	5			
1	J	222	Total	C	N	O	S	0	0	0
			1638	1027	282	324	5			
1	L	222	Total	C	N	O	S	0	0	0
			1638	1027	282	324	5			
1	N	223	Total	C	N	O	S	0	0	0
			1642	1029	283	325	5			
1	P	222	Total	C	N	O	S	0	0	0
			1638	1027	282	324	5			
1	R	222	Total	C	N	O	S	0	0	0
			1638	1027	282	324	5			
1	T	223	Total	C	N	O	S	0	0	0
			1642	1029	283	325	5			
1	V	226	Total	C	N	O	S	0	0	0
			1662	1040	286	331	5			
1	X	224	Total	C	N	O	S	0	0	0
			1647	1032	284	326	5			
1	Z	224	Total	C	N	O	S	0	0	0
			1647	1032	284	326	5			
1	2	222	Total	C	N	O	S	0	0	0
			1638	1027	282	324	5			

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	535	HIS	-	EXPRESSION TAG	UNP O33245

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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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 2 is a protein called Proteasome (Alpha subunit) PrcA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	213	Total	C	N	O	S	0	0	0
			1645	1030	301	310	4			
2	A	214	Total	C	N	O	S	0	0	0
			1653	1036	302	311	4			
2	B	214	Total	C	N	O	S	0	0	0
			1653	1036	302	311	4			
2	F	214	Total	C	N	O	S	0	0	0
			1653	1036	302	311	4			
2	I	214	Total	C	N	O	S	0	0	0
			1653	1036	302	311	4			
2	K	214	Total	C	N	O	S	0	0	0
			1653	1036	302	311	4			
2	M	214	Total	C	N	O	S	0	0	0
			1653	1036	302	311	4			
2	O	214	Total	C	N	O	S	0	0	0
			1653	1036	302	311	4			
2	Q	214	Total	C	N	O	S	0	0	0
			1653	1036	302	311	4			
2	S	214	Total	C	N	O	S	0	0	0
			1653	1036	302	311	4			
2	U	214	Total	C	N	O	S	0	0	0
			1653	1036	302	311	4			
2	W	214	Total	C	N	O	S	0	0	0
			1653	1036	302	311	4			
2	Y	214	Total	C	N	O	S	0	0	0
			1653	1036	302	311	4			
2	1	214	Total	C	N	O	S	0	0	0
			1653	1036	302	311	4			

There are 14 discrepancies between the modelled and reference sequences:

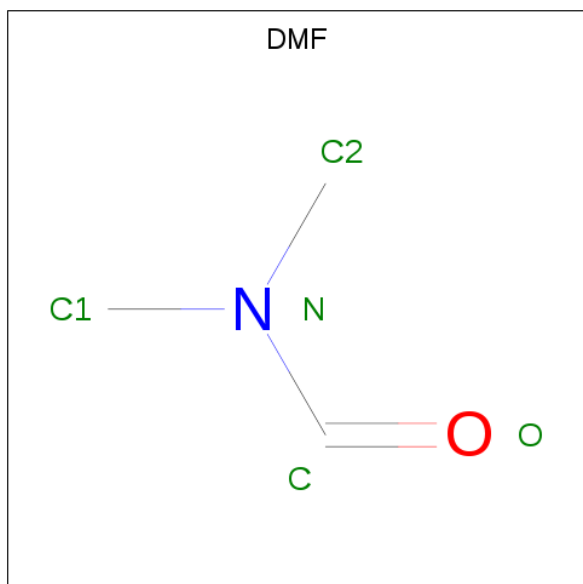
Chain	Residue	Modelled	Actual	Comment	Reference
D	9	MET	-	INITIATING METHIONINE	UNP O33244
A	9	MET	-	INITIATING METHIONINE	UNP O33244
B	9	MET	-	INITIATING METHIONINE	UNP O33244
F	9	MET	-	INITIATING METHIONINE	UNP O33244
I	9	MET	-	INITIATING METHIONINE	UNP O33244
K	9	MET	-	INITIATING METHIONINE	UNP O33244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

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Chain	Residue	Modelled	Actual	Comment	Reference
Y	9	MET	-	INITIATING METHIONINE	UNP O33244
1	9	MET	-	INITIATING METHIONINE	UNP O33244

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



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	C	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	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	J	1	Total	C	N	O	0	0
			5	3	1	1		

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

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	Z	1	Total 5	C 3	N 1	O 1	0	0
3	2	1	Total 5	C 3	N 1	O 1	0	0
3	2	1	Total 5	C 3	N 1	O 1	0	0
3	D	1	Total 5	C 3	N 1	O 1	0	0
3	A	1	Total 5	C 3	N 1	O 1	0	0
3	A	1	Total 5	C 3	N 1	O 1	0	0
3	B	1	Total 5	C 3	N 1	O 1	0	0
3	F	1	Total 5	C 3	N 1	O 1	0	0
3	I	1	Total 5	C 3	N 1	O 1	0	0
3	K	1	Total 5	C 3	N 1	O 1	0	0
3	K	1	Total 5	C 3	N 1	O 1	0	0
3	K	1	Total 5	C 3	N 1	O 1	0	0
3	M	1	Total 5	C 3	N 1	O 1	0	0
3	O	1	Total 5	C 3	N 1	O 1	0	0
3	Q	1	Total 5	C 3	N 1	O 1	0	0
3	Q	1	Total 5	C 3	N 1	O 1	0	0
3	Q	1	Total 5	C 3	N 1	O 1	0	0
3	S	1	Total 5	C 3	N 1	O 1	0	0
3	S	1	Total 5	C 3	N 1	O 1	0	0
3	U	1	Total 5	C 3	N 1	O 1	0	0
3	U	1	Total 5	C 3	N 1	O 1	0	0

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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	H	92	Total	O	0	0
			92	92		
4	C	43	Total	O	0	0
			43	43		
4	E	121	Total	O	0	0
			121	121		
4	G	113	Total	O	0	0
			113	113		
4	J	73	Total	O	0	0
			73	73		
4	L	109	Total	O	0	0
			109	109		
4	N	124	Total	O	0	0
			124	124		
4	P	93	Total	O	0	0
			93	93		
4	R	89	Total	O	0	0
			89	89		
4	T	96	Total	O	0	0
			96	96		
4	V	133	Total	O	0	0
			133	133		
4	X	101	Total	O	0	0
			101	101		
4	Z	91	Total	O	0	0
			91	91		


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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	2	107	Total 107	O 107	0	0
4	D	49	Total 49	O 49	0	0
4	A	31	Total 31	O 31	0	0
4	B	37	Total 37	O 37	0	0
4	F	60	Total 60	O 60	0	0
4	I	35	Total 35	O 35	0	0
4	K	52	Total 52	O 52	0	0
4	M	74	Total 74	O 74	0	0
4	O	34	Total 34	O 34	0	0
4	Q	71	Total 71	O 71	0	0
4	S	35	Total 35	O 35	0	0
4	U	48	Total 48	O 48	0	0
4	W	62	Total 62	O 62	0	0
4	Y	68	Total 68	O 68	0	0
4	1	68	Total 68	O 68	0	0

HIS
HIS
HIS
HIS
HIS
HIS


• Molecule 1: Proteasome (Beta subunit) PrcB

Chain J:  4% 84% 8% 8%

T301 L306 E362 L363 Y366 E367 K368 L374 R382 I385 L391 I409 H410 A411 S412 D413 P414 Q415 S416 L444 Q456 D461 R465 L471 D500 V503 P506 L513 A514 R515 E519 S522 GLY ALA ASP THR PHE GLY SER ASP GLY

GLY
GLU
LYS
HIS
HIS
HIS
HIS
HIS


• Molecule 1: Proteasome (Beta subunit) PrcB

Chain L:  2% 82% 10% 8%

T301 M325 D339 E362 L363 Y366 L374 T375 K379 R382 I385 L391 L398 I409 H410 A411 S412 D413 P414 Q415 S416 L444 Q456 D461 R465 L471 G482 G483 L513 E519 S522 GLY ALA ASP THR PHE GLY SER ASP GLY

GLY
GLU
LYS
HIS
HIS
HIS
HIS
HIS


• Molecule 1: Proteasome (Beta subunit) PrcB

Chain N:  83% 9% 7%

T301 L306 R332 E362 L363 Y366 L374 T375 R382 I385 R388 L398 I409 H410 A411 S412 D413 P414 W429 Q456 D461 R465 D473 D500 L513 B521 S522 G523 ALA ASP THR PHE GLY SER ASP GLY LYS HIS HIS

HIS
HIS
HIS


• Molecule 1: Proteasome (Beta subunit) PrcB

Chain P:  2% 84% 7% 8%

T301 E362 L363 Y366 L374 A377 N381 R382 I385 L391 Q396 I409 H410 A411 S412 D413 P414 Q415 L444 Q456 D461 R465 L471 L513 E519 S522 GLY ALA ASP THR PHE GLY SER ASP GLY GLY LYS HIS HIS HIS

HIS


• Molecule 1: Proteasome (Beta subunit) PrcB

Chain R:  82% 10% 8%

T301 L306 E362 L363 Y366 L374 R382 I385 L391 L401 P402 I409 H410 A411 S412 D413 P414 A417 W429 E432 E433 E434 L444 K451 R452 Q456 D461 R465 L471 B509 L513 S522 GLY ALA ASP THR PHE GLY SER

ASP
GLY
GLY
GLU
LYS
HIS
HIS
HIS
HIS
HIS


• Molecule 1: Proteasome (Beta subunit) PrcB

Chain T: 

T301 L306 E362 L363 Y366 L374 A377 R382 I385 L391 M395 L398 I409 H410 A411 S412 D413 P414 Q415 L444 Q456 D461 R465 L471 Y472 L513 G523 ALA ASP THR PHE GLY SER ASP GLY ASP GLY LYS HIS HIS HIS

HIS
HIS


• Molecule 1: Proteasome (Beta subunit) PrcB

Chain V: 

T301 R319 I345 R357 E362 L363 Y366 L374 T375 R382 I385 R388 I409 H410 A411 S412 D413 P414 W429 K451 Q456 D461 R465 L471 I496 L513 A514 R515 G523 T526 PHE GLY SER ASP GLY ASP GLY LYS HIS HIS HIS


HIS
HIS
HIS

• Molecule 1: Proteasome (Beta subunit) PrcB

Chain X: 


T301 M325 E362 L363 Y366 L374 R382 I385 L391 Q396 I409 H410 A411 S412 D413 P414 Q415 K451 Q456 D461 R465 L471 L513 G523 A524 ASP THR PHE GLY SER ASP GLY GLU LYS HIS HIS HIS

• Molecule 1: Proteasome (Beta subunit) PrcB

Chain Z: 

T301 R357 E362 L363 Y366 L374 R382 I385 L398 I409 H410 A411 S412 D413 P414 W429 L444 Q456 D461 R465 L471 I496 R509 L513 A524 ASP THR PHE GLY SER ASP GLY GLU LYS HIS HIS HIS

• Molecule 1: Proteasome (Beta subunit) PrcB

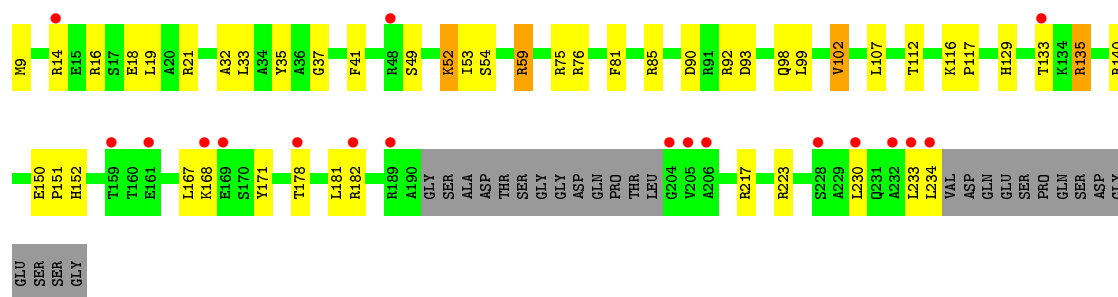
Chain 2: 

T301 L306 M325 E362 L363 Y366 L374 R382 I385 Q396 R397 L398 L401 P402 I409 H410 A411 S412 D413 P414 Q415 W429 S448 D461 L471 Y472 L513 G523 GLY ALA ASP THR PHE GLY SER ASP GLY ASP GLY LYS HIS HIS HIS

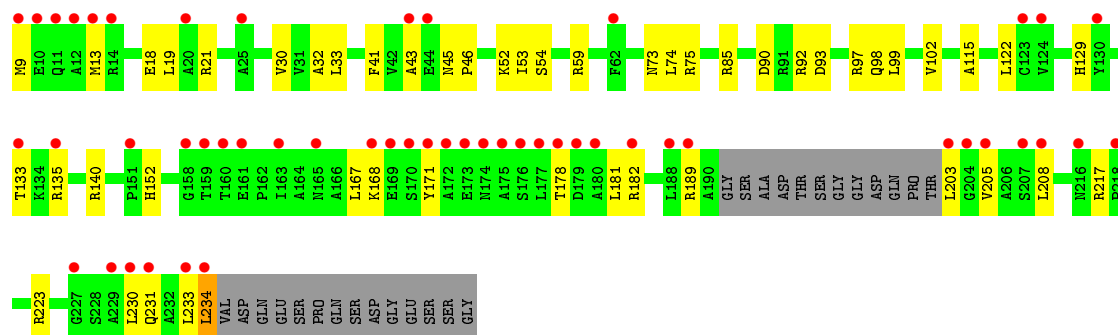
HIS
HIS

• Molecule 2: Proteasome (Alpha subunit) PrcA

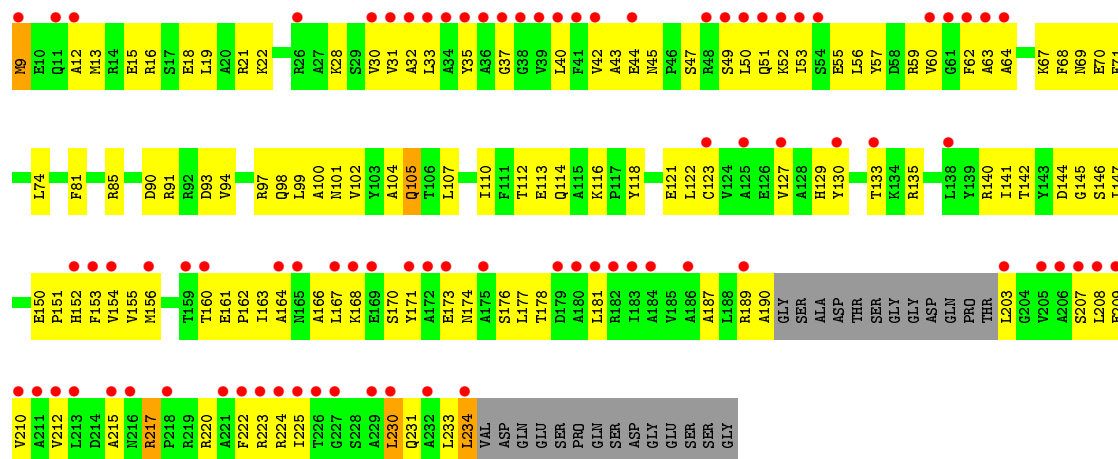
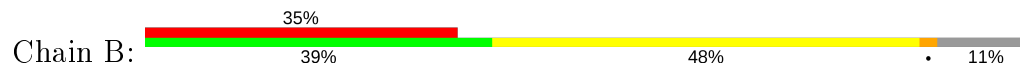
Chain D: 



• Molecule 2: Proteasome (Alpha subunit) PrcA

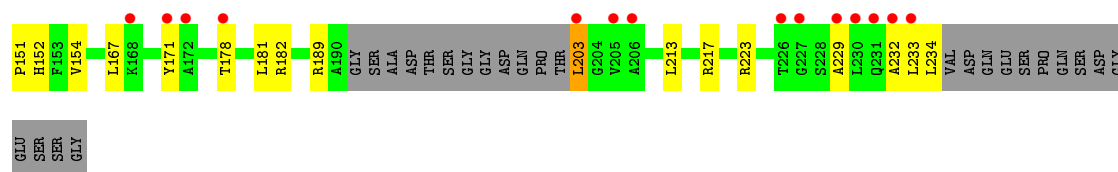


• Molecule 2: Proteasome (Alpha subunit) PrcA

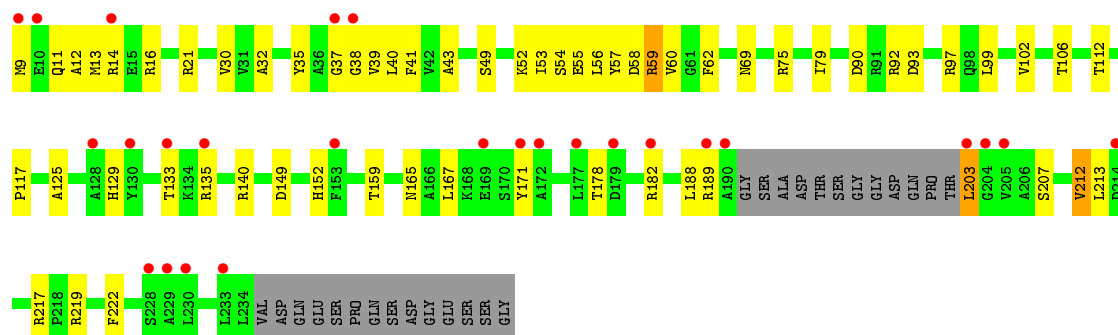


• Molecule 2: Proteasome (Alpha subunit) PrcA

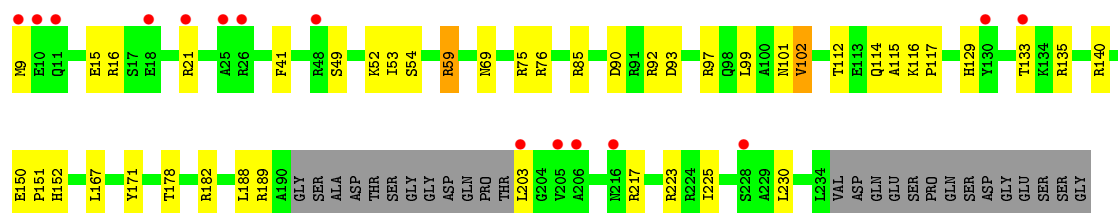




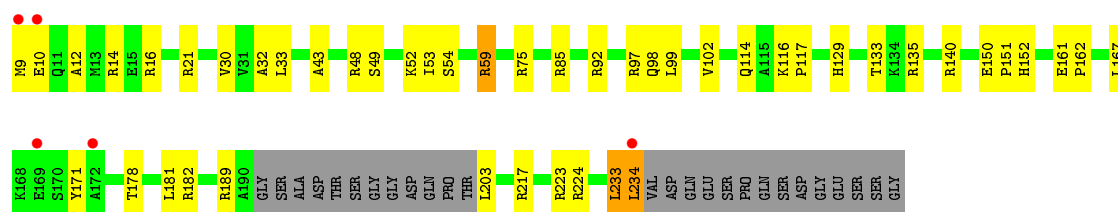
• Molecule 2: Proteasome (Alpha subunit) PrcA



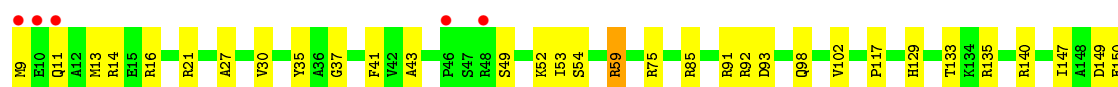
• Molecule 2: Proteasome (Alpha subunit) PrcA

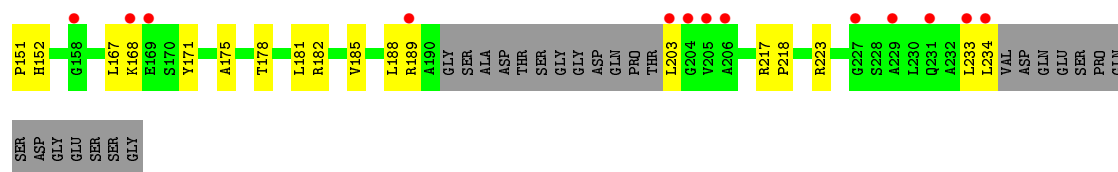


• Molecule 2: Proteasome (Alpha subunit) PrcA

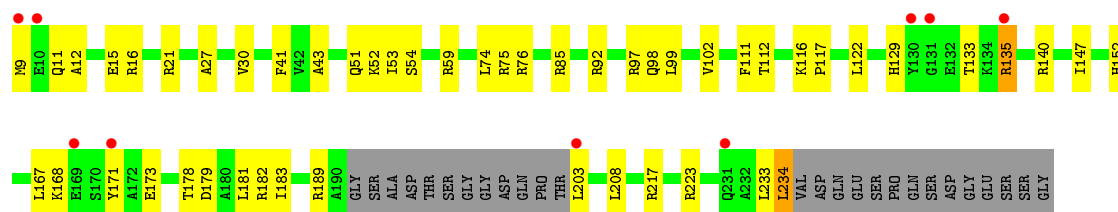


• Molecule 2: Proteasome (Alpha subunit) PrcA

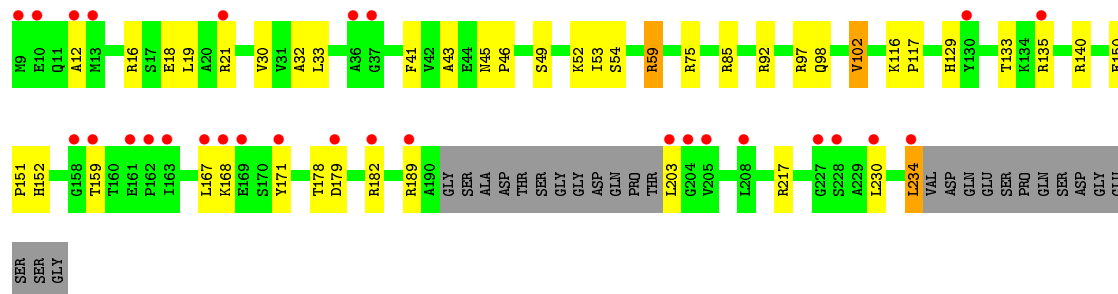




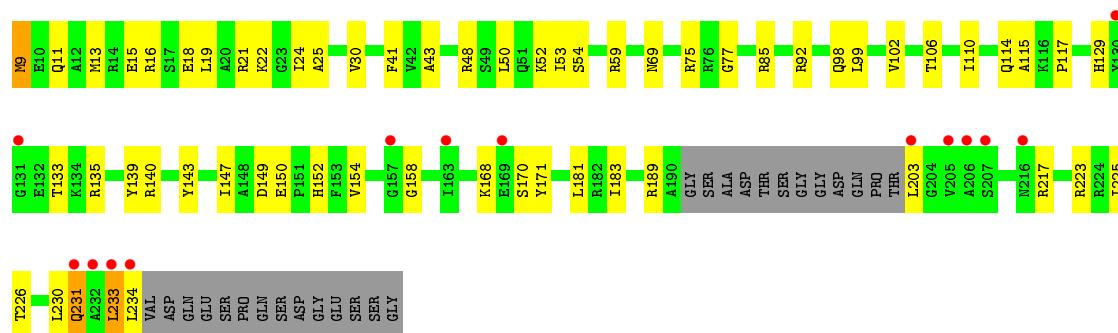
• Molecule 2: Proteasome (Alpha subunit) PrcA



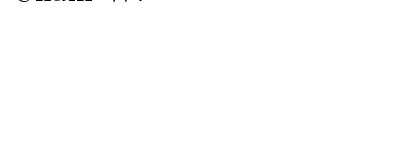
• Molecule 2: Proteasome (Alpha subunit) PrcA

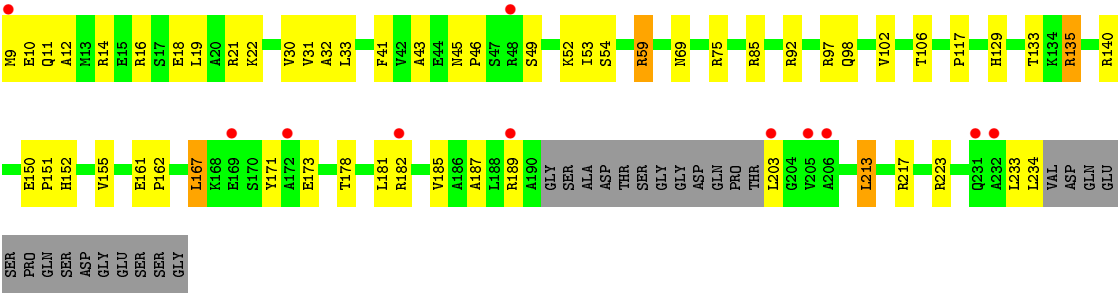


• Molecule 2: Proteasome (Alpha subunit) PrcA

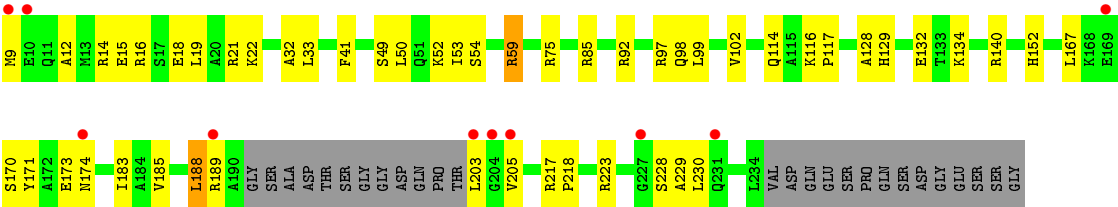


• Molecule 2: Proteasome (Alpha subunit) PrcA

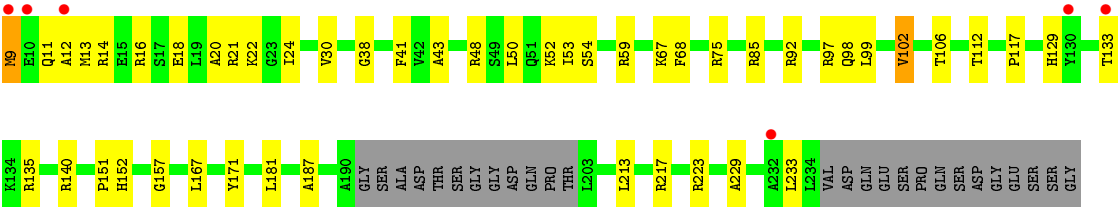




• Molecule 2: Proteasome (Alpha subunit) PrcA



• Molecule 2: Proteasome (Alpha subunit) PrcA



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	119.16Å 221.44Å 137.12Å 90.00° 104.89° 90.00°	Depositor
Resolution (Å)	29.86 – 2.50 29.86 – 2.50	Depositor EDS
% Data completeness (in resolution range)	97.8 (29.86-2.50) 97.8 (29.86-2.50)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.80 (at 2.51Å)	Xtriage
Refinement program	PHENIX (phenix.refine), CNS	Depositor
R, R_{free}	0.173 , 0.214 0.199 , 0.227	Depositor DCC
R_{free} test set	11458 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	33.3	Xtriage
Anisotropy	0.164	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 55.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	48523	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.15% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 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: 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	2	0.33	0/1662	0.49	0/2254
1	C	0.32	0/1662	0.50	0/2254
1	E	0.34	0/1666	0.49	0/2259
1	G	0.36	0/1662	0.50	0/2254
1	H	0.33	0/1666	0.48	0/2259
1	J	0.31	0/1662	0.48	0/2254
1	L	0.33	0/1662	0.49	0/2254
1	N	0.35	0/1666	0.49	0/2259
1	P	0.32	0/1662	0.49	0/2254
1	R	0.33	0/1662	0.49	0/2254
1	T	0.33	0/1666	0.49	0/2259
1	V	0.36	0/1686	0.50	0/2287
1	X	0.32	0/1671	0.49	0/2266
1	Z	0.32	0/1671	0.50	0/2266
2	1	0.32	0/1677	0.54	0/2264
2	A	0.32	0/1677	0.53	0/2264
2	B	0.32	0/1677	0.56	0/2264
2	D	0.36	0/1669	0.54	0/2253
2	F	0.32	0/1677	0.54	0/2264
2	I	0.32	0/1677	0.55	1/2264 (0.0%)
2	K	0.32	0/1677	0.53	0/2264
2	M	0.32	0/1677	0.54	0/2264
2	O	0.31	0/1677	0.51	0/2264
2	Q	0.33	0/1677	0.57	0/2264
2	S	0.29	0/1677	0.51	0/2264
2	U	0.32	0/1677	0.54	0/2264
2	W	0.33	0/1677	0.55	1/2264 (0.0%)
2	Y	0.33	0/1677	0.55	0/2264
All	All	0.33	0/46796	0.52	2/63318 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	I	213	LEU	N-CA-C	-5.19	96.99	111.00
2	W	213	LEU	N-CA-C	-5.11	97.20	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	2	1638	0	1630	16	0
1	C	1638	0	1630	23	0
1	E	1642	0	1633	28	0
1	G	1638	0	1630	21	0
1	H	1642	0	1633	15	0
1	J	1638	0	1630	15	0
1	L	1638	0	1630	21	0
1	N	1642	0	1633	19	0
1	P	1638	0	1630	18	0
1	R	1638	0	1630	23	0
1	T	1642	0	1633	19	0
1	V	1662	0	1649	22	0
1	X	1647	0	1638	16	0
1	Z	1647	0	1638	22	0
2	1	1653	0	1656	49	0
2	A	1653	0	1656	42	0
2	B	1653	0	1656	161	0
2	D	1645	0	1645	49	0
2	F	1653	0	1656	40	0
2	I	1653	0	1656	62	0
2	K	1653	0	1656	35	0
2	M	1653	0	1656	38	0
2	O	1653	0	1656	48	0
2	Q	1653	0	1656	39	0
2	S	1653	0	1656	51	0
2	U	1653	0	1656	47	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	W	1653	0	1656	52	0
2	Y	1653	0	1656	46	0
3	1	10	0	14	2	0
3	2	10	0	14	2	0
3	A	10	0	14	1	0
3	B	5	0	7	0	0
3	C	5	0	7	0	0
3	D	5	0	7	0	0
3	E	15	0	21	4	0
3	F	5	0	7	0	0
3	G	15	0	21	4	0
3	H	10	0	14	1	0
3	I	5	0	7	1	0
3	J	5	0	7	0	0
3	K	15	0	21	5	0
3	L	20	0	28	4	0
3	M	5	0	7	0	0
3	N	10	0	14	1	0
3	O	5	0	7	0	0
3	P	15	0	21	3	0
3	Q	15	0	21	5	0
3	S	10	0	14	1	0
3	T	10	0	14	5	0
3	U	10	0	14	1	0
3	V	25	0	35	7	0
3	W	5	0	7	1	0
3	X	5	0	7	0	0
3	Y	15	0	21	1	0
3	Z	25	0	35	7	0
4	1	68	0	0	1	0
4	2	107	0	0	3	0
4	A	31	0	0	0	0
4	B	37	0	0	4	0
4	C	43	0	0	1	0
4	D	49	0	0	5	0
4	E	121	0	0	8	0
4	F	60	0	0	4	0
4	G	113	0	0	2	0
4	H	92	0	0	0	0
4	I	35	0	0	6	0
4	J	73	0	0	2	0
4	K	52	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	L	109	0	0	4	0
4	M	74	0	0	5	0
4	N	124	0	0	6	0
4	O	34	0	0	4	0
4	P	93	0	0	2	0
4	Q	71	0	0	2	0
4	R	89	0	0	2	0
4	S	35	0	0	3	0
4	T	96	0	0	1	0
4	U	48	0	0	2	0
4	V	133	0	0	2	0
4	W	62	0	0	4	0
4	X	101	0	0	1	0
4	Y	68	0	0	3	0
4	Z	91	0	0	3	0
All	All	48523	0	46446	945	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 10.

All (945) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:115:ALA:HB3	2:B:112:THR:CG2	1.66	1.25
2:S:116:LYS:HB2	2:1:13:MET:CE	1.68	1.23
2:B:9:MET:CE	2:B:13:MET:HE3	1.68	1.22
2:S:230:LEU:O	2:S:234:LEU:HD13	1.34	1.22
2:O:9:MET:HE2	2:O:13:MET:CE	1.77	1.15
2:B:64:ALA:HB2	2:B:122:LEU:CD2	1.79	1.12
1:Z:509:ARG:HH12	3:Z:69:DMF:H23	1.15	1.11
2:B:217:ARG:HG2	2:B:217:ARG:HH11	1.16	1.10
2:A:115:ALA:HB3	2:B:112:THR:HG23	1.32	1.08
2:B:64:ALA:CB	2:B:122:LEU:HD23	1.84	1.08
2:O:9:MET:CE	2:O:13:MET:CE	2.33	1.07
2:B:9:MET:CE	2:B:13:MET:CE	2.33	1.05
2:D:16:ARG:HG2	2:K:9:MET:HE1	1.37	1.05
2:B:64:ALA:HB2	2:B:122:LEU:HD23	1.36	1.03
2:O:9:MET:CE	2:O:13:MET:HE3	1.88	1.02
2:B:9:MET:HE1	2:B:13:MET:HE3	1.41	1.02
2:S:116:LYS:HB2	2:1:13:MET:HE2	1.41	1.01
2:I:152:HIS:HB3	2:I:171:TYR:CE2	1.97	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:11:GLN:HA	2:I:11:GLN:OE1	1.57	0.99
2:I:11:GLN:HG3	2:I:14:ARG:NH1	1.79	0.98
2:S:116:LYS:HB2	2:I:13:MET:HE3	1.43	0.98
1:C:306:LEU:HD12	1:C:313:VAL:HG12	1.46	0.97
1:Z:496:ILE:HD12	3:Z:69:DMF:H22	1.46	0.97
2:B:35:TYR:CZ	2:B:177:LEU:HD13	1.99	0.96
2:B:181:LEU:HD23	2:B:181:LEU:O	1.66	0.95
2:B:217:ARG:HG3	2:B:223:ARG:HH21	1.29	0.95
2:B:35:TYR:OH	2:B:177:LEU:HD13	1.67	0.94
1:C:306:LEU:CD1	1:C:313:VAL:CG1	2.46	0.93
2:B:35:TYR:CZ	2:B:177:LEU:CD1	2.52	0.93
2:I:11:GLN:CG	2:I:14:ARG:NH1	2.32	0.93
2:W:181:LEU:O	2:W:181:LEU:HD23	1.69	0.92
2:O:9:MET:HE2	2:O:13:MET:HE2	1.48	0.92
2:O:9:MET:HE2	2:O:13:MET:HE3	1.42	0.92
2:B:31:VAL:CG1	2:B:33:LEU:HD11	2.02	0.89
2:B:181:LEU:HD23	2:B:181:LEU:C	1.93	0.88
2:I:11:GLN:HG3	2:I:14:ARG:HH12	1.37	0.88
2:A:115:ALA:CB	2:B:112:THR:HG23	2.04	0.87
2:B:155:VAL:HG11	2:B:164:ALA:HB2	1.54	0.87
2:B:189:ARG:HH21	2:B:203:LEU:HD22	1.40	0.87
2:D:35:TYR:CE1	2:D:37:GLY:HA3	2.09	0.87
2:D:16:ARG:HG2	2:K:9:MET:CE	2.03	0.87
1:C:306:LEU:HD11	1:C:313:VAL:CG1	2.04	0.87
2:B:217:ARG:HG2	2:B:217:ARG:NH1	1.87	0.86
2:B:9:MET:HE3	2:B:13:MET:HE3	1.57	0.86
2:I:35:TYR:CD2	2:I:38:GLY:O	2.30	0.85
1:C:306:LEU:CD1	1:C:313:VAL:HG12	2.05	0.85
2:M:59:ARG:HD2	2:M:129:HIS:HA	1.58	0.85
2:D:85:ARG:NH2	3:Q:251:DMF:H23	1.92	0.85
2:I:203:LEU:N	2:I:203:LEU:HD12	1.90	0.85
2:O:59:ARG:HD2	2:O:129:HIS:HA	1.58	0.85
2:B:64:ALA:CB	2:B:122:LEU:CD2	2.49	0.84
1:Z:509:ARG:NH1	3:Z:69:DMF:H23	1.92	0.84
2:F:59:ARG:HD2	2:F:129:HIS:HA	1.60	0.84
2:A:9:MET:CE	2:A:9:MET:HA	2.07	0.84
2:I:59:ARG:HD2	2:I:129:HIS:HA	1.58	0.84
2:K:59:ARG:HD2	2:K:129:HIS:HA	1.60	0.83
2:Q:59:ARG:HD2	2:Q:129:HIS:HA	1.61	0.83
2:D:14:ARG:HD3	4:D:1624:HOH:O	1.78	0.83
1:H:398:LEU:HD11	1:P:391:LEU:HD21	1.60	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:19:LEU:HD13	2:1:9:MET:CE	2.08	0.83
2:S:59:ARG:HD2	2:S:129:HIS:HA	1.60	0.82
2:Q:178:THR:O	2:Q:182:ARG:HG2	1.80	0.82
2:D:59:ARG:HD2	2:D:129:HIS:HA	1.60	0.82
2:B:49:SER:OG	2:I:97:ARG:HD2	1.78	0.82
2:S:230:LEU:CD1	2:S:234:LEU:HD11	2.10	0.82
2:U:59:ARG:HD2	2:U:129:HIS:HA	1.61	0.81
2:S:19:LEU:HD13	2:1:9:MET:HE3	1.63	0.81
2:1:59:ARG:HD2	2:1:129:HIS:HA	1.59	0.81
2:B:33:LEU:HG	2:B:153:PHE:HB2	1.62	0.81
2:A:59:ARG:HD2	2:A:129:HIS:HA	1.59	0.81
2:W:59:ARG:HD2	2:W:129:HIS:HA	1.62	0.81
2:B:30:VAL:HG12	2:B:43:ALA:CB	2.12	0.80
2:O:85:ARG:NH1	2:O:98:GLN:NE2	2.30	0.80
2:A:115:ALA:CB	2:B:112:THR:CG2	2.56	0.80
1:C:306:LEU:HD12	1:C:313:VAL:CG1	2.08	0.80
2:B:209:GLU:HB3	4:B:1703:HOH:O	1.80	0.79
2:O:35:TYR:CE1	2:O:37:GLY:HA3	2.17	0.79
2:W:189:ARG:HH12	2:W:203:LEU:N	1.81	0.78
1:T:395:MET:HE2	4:2:1676:HOH:O	1.84	0.78
1:T:472:TYR:CZ	3:T:62:DMF:H13	2.18	0.77
2:B:49:SER:HG	2:I:97:ARG:HD2	1.48	0.77
2:B:33:LEU:HG	2:B:153:PHE:CB	2.14	0.77
2:O:9:MET:HE1	2:O:13:MET:HE3	1.66	0.76
2:B:166:ALA:HB3	2:B:187:ALA:CB	2.16	0.76
2:S:230:LEU:HD12	2:S:234:LEU:HD11	1.66	0.76
2:W:181:LEU:C	2:W:181:LEU:HD23	2.06	0.76
2:B:19:LEU:O	2:B:19:LEU:HD23	1.85	0.76
3:H:142:DMF:HC	3:L:9:DMF:O	1.85	0.76
2:W:167:LEU:HD13	2:W:187:ALA:HB2	1.68	0.76
2:W:167:LEU:HD13	2:W:187:ALA:CB	2.16	0.75
2:B:47:SER:HB2	2:I:149:ASP:OD2	1.87	0.75
2:B:166:ALA:HB3	2:B:187:ALA:HB2	1.69	0.75
2:B:189:ARG:NH2	2:B:203:LEU:HD22	2.01	0.75
2:S:12:ALA:O	2:S:16:ARG:HG3	1.86	0.75
2:I:178:THR:HG22	2:I:182:ARG:HH21	1.52	0.74
2:Q:76:ARG:NH1	3:Q:251:DMF:H22	2.02	0.74
2:B:30:VAL:HG12	2:B:43:ALA:HB1	1.67	0.74
1:G:337:THR:HG21	1:G:359:TYR:HD2	1.52	0.74
2:D:99:LEU:O	2:D:102:VAL:HG12	1.88	0.74
1:H:362:GLU:OE2	1:H:382:ARG:HD3	1.88	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:18:GLU:CD	2:A:21:ARG:HH12	1.90	0.73
2:B:31:VAL:HG12	2:B:33:LEU:CD1	2.18	0.73
2:I:99:LEU:O	2:I:102:VAL:HG12	1.89	0.73
2:U:231:GLN:OE1	2:U:231:GLN:HA	1.86	0.73
2:B:31:VAL:CG1	2:B:33:LEU:CD1	2.67	0.72
2:B:231:GLN:O	2:B:234:LEU:HG	1.88	0.72
2:I:159:THR:HG23	2:I:159:THR:O	1.88	0.72
2:W:189:ARG:NH1	2:W:203:LEU:N	2.38	0.72
2:B:181:LEU:CD2	2:B:181:LEU:C	2.57	0.71
2:Y:203:LEU:HD12	2:Y:203:LEU:N	2.06	0.71
1:N:414:PRO:HD2	4:N:1177:HOH:O	1.89	0.71
2:U:85:ARG:NH1	2:U:98:GLN:NE2	2.38	0.71
2:W:152:HIS:HB3	2:W:171:TYR:CE2	2.25	0.71
2:A:205:VAL:HG21	2:A:231:GLN:OE1	1.89	0.71
2:B:59:ARG:HD2	2:B:127:VAL:HG13	1.71	0.70
2:O:9:MET:HE1	2:O:13:MET:CE	2.22	0.70
2:W:135:ARG:NH2	2:W:173:GLU:OE2	2.23	0.70
2:W:106:THR:HG21	3:W:249:DMF:HC	1.71	0.70
2:B:32:ALA:C	2:B:33:LEU:HD12	2.11	0.70
2:Q:152:HIS:HB3	2:Q:171:TYR:CE2	2.26	0.70
2:B:9:MET:HE2	2:B:13:MET:CE	2.20	0.69
2:1:18:GLU:HG3	2:1:22:LYS:HE3	1.74	0.69
2:I:11:GLN:HG2	2:I:14:ARG:NH1	2.06	0.69
2:A:115:ALA:HB3	2:B:112:THR:HG22	1.71	0.69
2:O:21:ARG:HB3	2:O:21:ARG:HH11	1.57	0.69
2:B:166:ALA:CB	2:B:187:ALA:HA	2.23	0.69
2:K:21:ARG:HB3	2:K:21:ARG:HH11	1.58	0.69
2:O:11:GLN:HG3	2:O:14:ARG:CZ	2.23	0.69
2:Q:97:ARG:HD2	2:Y:49:SER:HB2	1.75	0.69
2:D:21:ARG:NH1	2:D:21:ARG:HB3	2.09	0.68
2:O:21:ARG:HB3	2:O:21:ARG:NH1	2.09	0.68
2:S:21:ARG:HH11	2:S:21:ARG:HB3	1.58	0.68
2:S:21:ARG:NH1	2:S:21:ARG:HB3	2.09	0.68
2:D:21:ARG:HH11	2:D:21:ARG:HB3	1.58	0.67
2:W:30:VAL:HG13	2:W:43:ALA:HB2	1.76	0.67
1:T:362:GLU:OE2	1:T:382:ARG:HD3	1.94	0.67
2:I:189:ARG:NH1	2:I:203:LEU:N	2.42	0.67
2:Q:12:ALA:O	2:Q:16:ARG:HG3	1.95	0.67
2:K:21:ARG:HB3	2:K:21:ARG:NH1	2.09	0.67
2:F:21:ARG:HB3	2:F:21:ARG:NH1	2.10	0.67
2:S:116:LYS:CB	2:1:13:MET:HE2	2.23	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:92:ARG:HD3	2:M:129:HIS:CE1	2.30	0.67
2:B:166:ALA:O	2:B:170:SER:HB3	1.93	0.66
1:Z:362:GLU:OE2	1:Z:382:ARG:HD3	1.95	0.66
2:B:164:ALA:O	2:B:168:LYS:HB2	1.95	0.66
2:S:116:LYS:CB	2:I:13:MET:HE3	2.23	0.66
2:F:21:ARG:HH11	2:F:21:ARG:HB3	1.61	0.66
2:S:117:PRO:HD2	2:I:9:MET:HE1	1.77	0.66
2:Y:16:ARG:NH2	2:Y:114:GLN:O	2.23	0.66
2:W:178:THR:HG22	2:W:182:ARG:HH21	1.60	0.66
2:B:189:ARG:HA	2:B:189:ARG:NE	2.10	0.66
2:B:225:ILE:O	2:B:225:ILE:HG13	1.94	0.66
2:M:21:ARG:NH1	2:M:21:ARG:HB3	2.11	0.66
2:F:178:THR:HG22	2:F:182:ARG:HH21	1.61	0.66
2:I:21:ARG:HH11	2:I:21:ARG:HB3	1.61	0.66
2:I:21:ARG:HB3	2:I:21:ARG:NH1	2.11	0.66
2:I:92:ARG:HD3	2:I:129:HIS:CE1	2.31	0.66
2:K:178:THR:HG22	2:K:182:ARG:HH21	1.61	0.66
2:M:21:ARG:HH11	2:M:21:ARG:HB3	1.60	0.66
2:A:178:THR:HG22	2:A:182:ARG:HH21	1.61	0.65
1:C:306:LEU:HD11	1:C:313:VAL:HG11	1.76	0.65
2:U:9:MET:HE1	2:U:13:MET:CE	2.26	0.65
2:O:178:THR:HG22	2:O:182:ARG:HH21	1.61	0.65
2:W:19:LEU:HD23	2:W:19:LEU:C	2.16	0.65
2:K:15:GLU:OE1	2:M:9:MET:N	2.30	0.65
2:U:92:ARG:HD3	2:U:129:HIS:CE1	2.32	0.65
2:A:90:ASP:HB3	2:A:93:ASP:OD2	1.95	0.65
1:X:362:GLU:OE2	1:X:382:ARG:HD3	1.96	0.65
2:Q:189:ARG:HH12	2:Q:203:LEU:N	1.95	0.65
2:Q:21:ARG:HB3	2:Q:21:ARG:NH1	2.12	0.65
2:W:11:GLN:OE1	2:W:14:ARG:NH1	2.30	0.65
2:B:9:MET:HE3	2:B:13:MET:CE	2.18	0.65
2:B:15:GLU:CD	2:I:9:MET:N	2.50	0.65
1:N:362:GLU:OE2	1:N:382:ARG:HD3	1.96	0.65
2:Y:128:ALA:HB1	2:Y:132:GLU:HG3	1.78	0.65
2:B:121:GLU:OE2	2:B:140:ARG:NH1	2.30	0.64
2:B:163:ILE:O	2:B:187:ALA:HB1	1.97	0.64
2:D:85:ARG:HH21	3:Q:251:DMF:H23	1.60	0.64
2:B:33:LEU:HD21	2:B:167:LEU:HD13	1.78	0.64
2:Q:21:ARG:HH11	2:Q:21:ARG:HB3	1.62	0.64
2:B:31:VAL:HG11	2:B:33:LEU:HD11	1.77	0.64
1:R:362:GLU:OE2	1:R:382:ARG:HD3	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:229:ALA:O	2:1:233:LEU:HD13	1.97	0.64
2:B:35:TYR:OH	2:B:177:LEU:CD1	2.40	0.64
2:F:92:ARG:HD3	2:F:129:HIS:CE1	2.32	0.64
2:M:178:THR:HG22	2:M:182:ARG:HH21	1.63	0.64
2:I:106:THR:HG21	3:I:249:DMF:HC	1.79	0.64
2:U:9:MET:CE	2:U:13:MET:CE	2.76	0.64
2:1:181:LEU:HD23	2:1:233:LEU:HB3	1.80	0.64
1:G:362:GLU:OE2	1:G:382:ARG:HD3	1.97	0.64
1:X:391:LEU:HD21	1:Z:398:LEU:HD11	1.80	0.64
1:T:391:LEU:HD21	1:2:398:LEU:HD11	1.79	0.64
2:D:90:ASP:HB3	2:D:93:ASP:OD2	1.98	0.64
1:E:362:GLU:OE2	1:E:382:ARG:HD3	1.98	0.64
2:Y:152:HIS:HB3	2:Y:171:TYR:CE2	2.33	0.64
2:D:178:THR:HG22	2:D:182:ARG:HH21	1.61	0.63
2:I:165:ASN:ND2	4:I:1026:HOH:O	2.30	0.63
2:F:97:ARG:HD2	2:M:49:SER:HB2	1.80	0.63
1:T:382:ARG:NH2	1:T:385:ILE:HD13	2.13	0.63
2:B:35:TYR:CZ	2:B:177:LEU:HD12	2.31	0.63
2:O:11:GLN:NE2	4:O:2134:HOH:O	2.30	0.63
2:O:85:ARG:HH12	2:O:98:GLN:NE2	1.96	0.63
1:H:398:LEU:HD11	1:P:391:LEU:CD2	2.29	0.63
2:M:161:GLU:HB3	2:M:162:PRO:HD3	1.79	0.63
1:V:362:GLU:OE2	1:V:382:ARG:HD3	1.98	0.63
2:1:92:ARG:HD3	2:1:129:HIS:CE1	2.33	0.63
2:B:19:LEU:C	2:B:19:LEU:HD23	2.18	0.63
1:C:362:GLU:OE2	1:C:382:ARG:HD3	1.99	0.63
2:B:47:SER:CB	4:I:1752:HOH:O	2.47	0.63
1:E:382:ARG:NH2	1:E:385:ILE:HD13	2.13	0.63
2:M:85:ARG:HH12	2:M:98:GLN:NE2	1.96	0.63
1:R:382:ARG:NH2	1:R:385:ILE:HD13	2.13	0.63
2:Y:189:ARG:NH1	2:Y:203:LEU:HD12	2.14	0.63
2:S:159:THR:HA	4:S:1892:HOH:O	1.98	0.63
2:K:92:ARG:HD3	2:K:129:HIS:CE1	2.34	0.63
2:O:151:PRO:HD2	4:O:249:HOH:O	1.97	0.63
2:B:123:CYS:SG	2:B:154:VAL:HG21	2.39	0.63
2:B:217:ARG:CG	2:B:223:ARG:HH21	2.08	0.63
2:D:92:ARG:HD3	2:D:129:HIS:CE1	2.34	0.63
2:S:116:LYS:CB	2:1:13:MET:CE	2.62	0.62
2:I:152:HIS:CB	2:I:171:TYR:CE2	2.80	0.62
2:D:16:ARG:CG	2:K:9:MET:HE1	2.22	0.62
2:Q:85:ARG:HH12	2:Q:98:GLN:NE2	1.96	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:85:ARG:HH12	2:S:98:GLN:NE2	1.96	0.62
1:V:366:TYR:CD2	1:V:374:LEU:HD13	2.35	0.62
2:A:92:ARG:HD3	2:A:129:HIS:CE1	2.34	0.62
2:W:85:ARG:HH12	2:W:98:GLN:NE2	1.98	0.62
2:W:18:GLU:OE2	2:W:21:ARG:NH1	2.30	0.62
1:P:362:GLU:OE2	1:P:382:ARG:HD3	1.98	0.62
2:Q:152:HIS:HB3	2:Q:171:TYR:CZ	2.35	0.62
2:O:149:ASP:OD2	2:U:48:ARG:HG2	1.99	0.62
2:W:181:LEU:C	2:W:181:LEU:CD2	2.68	0.62
2:D:81:PHE:HE2	2:D:98:GLN:HE21	1.47	0.62
2:A:203:LEU:HD23	2:A:208:LEU:HD21	1.80	0.62
2:B:152:HIS:HB3	2:B:171:TYR:CZ	2.35	0.62
1:G:429:TRP:CH2	3:G:140:DMF:H13	2.35	0.62
2:S:92:ARG:HD3	2:S:129:HIS:CE1	2.35	0.62
2:W:92:ARG:HD3	2:W:129:HIS:CE1	2.35	0.62
1:2:362:GLU:OE2	1:2:382:ARG:HD3	1.99	0.62
2:U:11:GLN:O	2:U:15:GLU:HG3	2.00	0.62
2:S:19:LEU:HD13	2:1:9:MET:HE1	1.80	0.61
2:W:12:ALA:O	2:W:16:ARG:HG3	1.99	0.61
2:Y:59:ARG:HD2	2:Y:129:HIS:HA	1.81	0.61
2:Y:85:ARG:HH12	2:Y:98:GLN:NE2	1.98	0.61
2:B:217:ARG:HD3	2:B:220:ARG:O	2.00	0.61
2:I:203:LEU:N	2:I:203:LEU:CD1	2.63	0.61
2:O:92:ARG:HD3	2:O:129:HIS:CE1	2.35	0.61
2:1:12:ALA:O	2:1:16:ARG:HG3	2.01	0.61
2:A:205:VAL:CG2	2:A:231:GLN:OE1	2.47	0.61
1:L:362:GLU:OE2	1:L:382:ARG:HD3	2.01	0.61
2:1:18:GLU:OE2	2:1:21:ARG:NH2	2.30	0.61
1:X:456:GLN:HE22	1:X:465:ARG:NH2	1.99	0.61
2:B:166:ALA:HB3	2:B:187:ALA:CA	2.30	0.61
2:S:234:LEU:N	2:S:234:LEU:CD1	2.63	0.61
2:U:85:ARG:NH1	2:U:98:GLN:HE22	1.97	0.61
2:Y:152:HIS:HB3	2:Y:171:TYR:CZ	2.35	0.61
2:D:35:TYR:CE1	2:D:37:GLY:CA	2.81	0.61
1:H:382:ARG:NH2	1:H:385:ILE:HD13	2.15	0.61
1:C:382:ARG:NH2	1:C:385:ILE:HD13	2.16	0.61
1:L:444:LEU:HB2	4:L:290:HOH:O	2.01	0.61
1:Z:509:ARG:HH12	3:Z:69:DMF:C2	2.04	0.61
2:B:47:SER:HB3	4:I:1752:HOH:O	2.00	0.60
2:B:166:ALA:HB3	2:B:187:ALA:HA	1.82	0.60
2:B:68:PHE:HA	2:B:71:PHE:CE2	2.36	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:391:LEU:HD21	1:N:398:LEU:HD11	1.83	0.60
2:Q:92:ARG:HD3	2:Q:129:HIS:CE1	2.36	0.60
2:B:127:VAL:CG2	2:B:215:ALA:HB2	2.30	0.60
2:B:127:VAL:HG21	2:B:215:ALA:HB2	1.83	0.60
2:D:135:ARG:NH1	4:D:2073:HOH:O	2.32	0.60
2:S:117:PRO:CD	2:I:9:MET:CE	2.78	0.60
1:R:366:TYR:CD2	1:R:374:LEU:HD13	2.36	0.60
1:V:382:ARG:NH2	1:V:385:ILE:HD13	2.16	0.60
2:A:85:ARG:HH12	2:A:98:GLN:NE2	2.00	0.60
1:C:456:GLN:HE22	1:C:465:ARG:NH2	2.00	0.60
2:B:152:HIS:HB3	2:B:171:TYR:CE2	2.37	0.60
2:U:25:ALA:O	2:U:158:GLY:HA2	2.02	0.60
2:K:90:ASP:HB3	2:K:93:ASP:OD2	2.02	0.60
3:V:16:DMF:HC	4:2:554:HOH:O	2.01	0.60
2:A:9:MET:HE1	2:A:9:MET:HA	1.84	0.59
1:J:456:GLN:HE22	1:J:465:ARG:NH2	1.99	0.59
1:N:382:ARG:NH2	1:N:385:ILE:HD13	2.17	0.59
2:Q:203:LEU:HD13	2:Q:208:LEU:HD21	1.84	0.59
2:S:49:SER:HB2	2:I:97:ARG:HD2	1.83	0.59
2:U:15:GLU:O	2:U:18:GLU:HG2	2.03	0.59
1:V:429:TRP:CZ2	3:V:121:DMF:H22	2.36	0.59
2:W:49:SER:HB2	2:Y:97:ARG:HD2	1.83	0.59
1:E:380:ILE:HB	3:E:104:DMF:H13	1.85	0.59
1:H:366:TYR:CD2	1:H:374:LEU:HD13	2.38	0.59
1:J:362:GLU:OE2	1:J:382:ARG:HD3	2.01	0.59
2:U:77:GLY:HA3	3:U:249:DMF:O	2.01	0.59
2:B:35:TYR:CE1	2:B:37:GLY:HA3	2.37	0.59
1:G:448:SER:HB3	1:2:448:SER:HB3	1.83	0.59
1:X:382:ARG:NH2	1:X:385:ILE:HD13	2.17	0.59
2:B:49:SER:OG	2:I:97:ARG:CD	2.51	0.59
2:I:59:ARG:NH2	2:I:217:ARG:O	2.35	0.59
1:P:396:GLN:NE2	4:P:1778:HOH:O	2.35	0.59
2:S:230:LEU:HD12	2:S:234:LEU:CD1	2.33	0.59
2:M:181:LEU:HD23	2:M:233:LEU:HB3	1.84	0.59
2:B:40:LEU:HA	2:B:212:VAL:HG12	1.84	0.59
2:B:85:ARG:HB3	2:B:93:ASP:OD2	2.02	0.59
2:B:33:LEU:HD21	2:B:167:LEU:HD22	1.85	0.58
1:X:366:TYR:CD2	1:X:374:LEU:HD13	2.38	0.58
2:Y:205:VAL:HG13	2:Y:230:LEU:HD23	1.84	0.58
2:B:64:ALA:HB1	2:B:122:LEU:HD23	1.81	0.58
2:B:18:GLU:HA	2:B:21:ARG:HG2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:11:GLN:HG3	2:I:14:ARG:CZ	2.33	0.58
1:J:382:ARG:NH2	1:J:385:ILE:HD13	2.17	0.58
1:P:456:GLN:HE22	1:P:465:ARG:NH2	2.00	0.58
2:S:230:LEU:HD11	2:S:234:LEU:HD11	1.86	0.58
2:B:97:ARG:O	2:B:101:ASN:HB2	2.03	0.58
1:H:456:GLN:HE22	1:H:465:ARG:NH2	2.01	0.58
1:P:382:ARG:NH2	1:P:385:ILE:HD13	2.19	0.58
1:T:456:GLN:HE22	1:T:465:ARG:NH2	2.01	0.58
2:F:85:ARG:HH12	2:F:98:GLN:NE2	2.02	0.58
2:W:18:GLU:O	2:W:22:LYS:HG3	2.04	0.58
2:U:9:MET:HG3	2:1:16:ARG:HG2	1.86	0.58
1:Z:456:GLN:HE22	1:Z:465:ARG:NH2	2.01	0.58
2:O:9:MET:CE	2:O:13:MET:HE2	2.18	0.58
1:V:366:TYR:CE2	1:V:374:LEU:HD13	2.38	0.58
3:Y:249:DMF:H21	4:Y:944:HOH:O	2.03	0.58
2:B:28:LYS:HE3	2:B:44:GLU:HB3	1.85	0.58
2:I:178:THR:CG2	2:I:182:ARG:HH21	2.17	0.58
2:B:45:ASN:ND2	2:B:50:LEU:O	2.36	0.57
1:E:456:GLN:HE22	1:E:465:ARG:NH2	2.01	0.57
2:F:189:ARG:HH12	2:F:203:LEU:N	2.02	0.57
1:G:337:THR:HG21	1:G:359:TYR:CD2	2.37	0.57
2:M:189:ARG:NH1	4:M:1093:HOH:O	2.33	0.57
2:W:161:GLU:HB3	2:W:162:PRO:HD3	1.86	0.57
1:Z:382:ARG:NH2	1:Z:385:ILE:HD13	2.19	0.57
2:M:10:GLU:O	2:M:14:ARG:HB2	2.05	0.57
2:A:9:MET:HE2	2:A:9:MET:HA	1.87	0.57
1:N:456:GLN:HE22	1:N:465:ARG:NH2	2.02	0.57
2:B:142:THR:CG2	2:B:146:SER:HB2	2.34	0.57
2:B:121:GLU:HG2	2:B:156:MET:HG2	1.85	0.57
2:S:59:ARG:NH2	2:S:217:ARG:O	2.36	0.57
2:S:117:PRO:HD3	2:1:9:MET:CE	2.34	0.57
1:N:366:TYR:CD2	1:N:374:LEU:HD13	2.39	0.57
1:P:366:TYR:CD2	1:P:374:LEU:HD13	2.39	0.57
2:D:85:ARG:NH2	3:Q:251:DMF:C2	2.65	0.57
2:S:234:LEU:HD12	2:S:234:LEU:N	2.18	0.57
2:1:85:ARG:HH12	2:1:98:GLN:NE2	2.03	0.57
2:B:178:THR:OG1	2:B:233:LEU:HD11	2.03	0.57
1:R:456:GLN:HE22	1:R:465:ARG:NH2	2.03	0.57
2:I:189:ARG:HH12	2:I:203:LEU:N	2.02	0.57
1:L:382:ARG:NH2	1:L:385:ILE:HD13	2.19	0.57
1:L:456:GLN:HE22	1:L:465:ARG:NH2	2.01	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:56:LEU:HD13	2:I:99:LEU:HD13	1.86	0.56
2:K:85:ARG:NH2	3:K:251:DMF:C1	2.68	0.56
1:V:375:THR:HG23	2:O:93:ASP:OD1	2.05	0.56
1:G:429:TRP:CZ2	3:G:140:DMF:H22	2.39	0.56
4:U:1698:HOH:O	2:1:67:LYS:HE3	2.06	0.56
2:B:30:VAL:HG12	2:B:43:ALA:HB2	1.85	0.56
2:D:151:PRO:HD2	4:D:1854:HOH:O	2.05	0.56
2:F:48:ARG:HD2	4:F:1871:HOH:O	2.05	0.56
1:G:456:GLN:HE22	1:G:465:ARG:NH2	2.02	0.56
2:O:85:ARG:NH1	2:O:98:GLN:HE22	2.02	0.56
2:K:85:ARG:NH2	3:K:251:DMF:H11	2.21	0.56
2:M:181:LEU:HD21	2:M:234:LEU:CD1	2.35	0.56
2:B:18:GLU:OE2	2:B:21:ARG:HD3	2.06	0.56
1:E:465:ARG:NH2	4:E:1535:HOH:O	2.38	0.56
2:D:18:GLU:OE2	2:D:21:ARG:NH1	2.39	0.56
2:B:33:LEU:HG	2:B:153:PHE:HB3	1.87	0.56
1:G:382:ARG:NH2	1:G:385:ILE:HD13	2.20	0.56
1:V:523:GLY:O	1:V:526:THR:HG22	2.05	0.56
2:B:35:TYR:CE1	2:B:177:LEU:HD13	2.39	0.56
1:G:366:TYR:CD2	1:G:374:LEU:HD13	2.41	0.56
1:L:366:TYR:CD2	1:L:374:LEU:HD13	2.41	0.56
2:U:139:TYR:CD1	2:U:149:ASP:HB3	2.41	0.56
1:V:429:TRP:CH2	3:V:121:DMF:H13	2.41	0.56
2:B:173:GLU:HG2	2:B:174:ASN:ND2	2.20	0.56
2:B:74:LEU:HD13	2:B:122:LEU:HD11	1.88	0.56
2:F:49:SER:HB2	2:W:97:ARG:HD2	1.88	0.56
1:J:366:TYR:CD2	1:J:374:LEU:HD13	2.41	0.56
2:Y:18:GLU:OE1	2:Y:21:ARG:NH1	2.30	0.56
2:Q:181:LEU:HD23	2:Q:233:LEU:HB3	1.87	0.55
1:2:382:ARG:NH2	1:2:385:ILE:HD13	2.21	0.55
1:G:444:LEU:HD21	1:X:325:MET:SD	2.47	0.55
1:G:465:ARG:NH1	4:G:2051:HOH:O	2.39	0.55
2:I:152:HIS:CG	2:I:171:TYR:HE2	2.24	0.55
2:I:90:ASP:HB3	2:I:93:ASP:OD2	2.06	0.55
2:S:85:ARG:NH1	2:S:98:GLN:NE2	2.54	0.55
1:N:500:ASP:HB2	4:N:1447:HOH:O	2.06	0.55
2:O:35:TYR:CE1	2:O:37:GLY:CA	2.90	0.55
1:V:456:GLN:HE22	1:V:465:ARG:NH2	2.04	0.55
1:Z:496:ILE:HD12	3:Z:69:DMF:C2	2.29	0.55
2:1:167:LEU:HG	2:1:187:ALA:CB	2.37	0.55
2:A:33:LEU:N	2:A:33:LEU:HD12	2.22	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:366:TYR:CD2	1:Z:374:LEU:HD13	2.42	0.55
2:D:16:ARG:CG	2:K:9:MET:CE	2.82	0.54
2:1:11:GLN:OE1	2:1:14:ARG:NE	2.40	0.54
2:B:55:GLU:HB3	2:B:222:PHE:CG	2.42	0.54
2:B:68:PHE:HA	2:B:71:PHE:CZ	2.42	0.54
1:E:380:ILE:HB	3:E:104:DMF:C1	2.36	0.54
1:E:366:TYR:CD2	1:E:374:LEU:HD13	2.42	0.54
1:C:366:TYR:CD2	1:C:374:LEU:HD13	2.42	0.54
2:B:62:PHE:CZ	2:B:122:LEU:HD22	2.43	0.54
1:E:465:ARG:NH1	4:E:1397:HOH:O	2.39	0.54
2:M:85:ARG:NH1	2:M:98:GLN:NE2	2.55	0.54
2:Y:189:ARG:HH12	2:Y:203:LEU:N	2.05	0.54
2:F:151:PRO:HD2	4:F:729:HOH:O	2.07	0.54
2:B:31:VAL:HG11	2:B:167:LEU:HD11	1.89	0.54
2:Q:11:GLN:HA	2:Q:11:GLN:NE2	2.22	0.54
1:R:366:TYR:CE2	1:R:374:LEU:HD13	2.42	0.54
2:B:32:ALA:HB3	2:B:154:VAL:CG2	2.38	0.54
2:O:85:ARG:NH1	2:O:98:GLN:HE21	2.02	0.54
1:V:319:ARG:HH22	3:V:135:DMF:H11	1.72	0.54
2:W:16:ARG:HB3	2:W:117:PRO:HG3	1.88	0.54
2:I:49:SER:HB2	2:S:97:ARG:HD2	1.90	0.54
4:N:1268:HOH:O	1:V:451:LYS:HE3	2.08	0.54
2:B:112:THR:HG22	2:B:113:GLU:HG3	1.90	0.54
1:E:325:MET:SD	1:R:444:LEU:HD21	2.48	0.54
2:D:116:LYS:HG3	2:D:117:PRO:HD2	1.90	0.53
2:W:9:MET:HG2	2:W:9:MET:O	2.09	0.53
2:Q:112:THR:HG21	2:Y:116:LYS:HE3	1.90	0.53
2:1:11:GLN:OE1	2:1:11:GLN:CA	2.40	0.53
1:2:366:TYR:CD2	1:2:374:LEU:HD13	2.43	0.53
2:A:74:LEU:HD13	2:A:122:LEU:HD11	1.89	0.53
2:Q:16:ARG:HB3	2:Q:117:PRO:HG3	1.91	0.53
2:W:18:GLU:HG3	2:W:22:LYS:HE3	1.88	0.53
2:Y:12:ALA:O	2:Y:16:ARG:HG3	2.09	0.53
2:Y:170:SER:OG	2:Y:183:ILE:HG23	2.08	0.53
2:A:152:HIS:HB3	2:A:171:TYR:CE2	2.44	0.53
1:E:366:TYR:CE2	1:E:374:LEU:HD13	2.43	0.53
1:T:377:ALA:HB1	3:T:134:DMF:H13	1.91	0.53
1:L:483:GLY:HA2	4:L:789:HOH:O	2.08	0.53
2:Q:11:GLN:HE21	2:Q:11:GLN:HA	1.73	0.53
2:Y:97:ARG:NH1	4:Y:849:HOH:O	2.42	0.53
2:Q:85:ARG:NH1	2:Q:98:GLN:NE2	2.56	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:152:HIS:HB3	2:W:171:TYR:CZ	2.43	0.53
2:B:63:ALA:HB3	2:B:123:CYS:HB3	1.89	0.53
1:T:366:TYR:CD2	1:T:374:LEU:HD13	2.44	0.53
2:D:76:ARG:HD3	4:D:252:HOH:O	2.09	0.52
2:U:18:GLU:O	2:U:22:LYS:HG3	2.09	0.52
2:W:11:GLN:OE1	2:W:14:ARG:CZ	2.57	0.52
2:I:40:LEU:HA	2:I:212:VAL:HG12	1.91	0.52
2:S:19:LEU:HD23	2:S:19:LEU:C	2.29	0.52
2:W:85:ARG:NH1	2:W:98:GLN:NE2	2.58	0.52
2:S:117:PRO:CD	2:1:9:MET:HE2	2.38	0.52
2:I:60:VAL:HG11	2:I:99:LEU:HD12	1.91	0.52
2:Q:217:ARG:HH11	2:Q:223:ARG:HD3	1.74	0.52
2:I:178:THR:HG22	2:I:182:ARG:NH2	2.21	0.52
2:S:116:LYS:HG3	2:1:9:MET:HE1	1.91	0.52
2:A:19:LEU:C	2:A:19:LEU:HD23	2.30	0.52
2:M:10:GLU:O	2:M:14:ARG:CB	2.58	0.52
2:U:150:GLU:HG3	2:U:154:VAL:HG22	1.91	0.52
2:U:217:ARG:HH11	2:U:223:ARG:HD3	1.75	0.52
2:1:20:ALA:O	2:1:24:ILE:HG13	2.09	0.52
2:B:155:VAL:HG11	2:B:164:ALA:CB	2.33	0.52
2:K:189:ARG:HH12	2:K:203:LEU:N	2.08	0.52
1:E:329:ARG:HD2	1:R:434:GLU:OE1	2.09	0.52
2:Y:14:ARG:O	2:Y:18:GLU:HG2	2.09	0.52
2:B:162:PRO:HB2	2:B:190:ALA:HB1	1.92	0.52
1:R:465:ARG:NH1	4:R:2061:HOH:O	2.43	0.52
2:W:217:ARG:HH11	2:W:223:ARG:HD3	1.75	0.52
2:F:181:LEU:HD23	2:F:233:LEU:HB3	1.91	0.52
2:F:9:MET:O	2:F:9:MET:HG2	2.09	0.52
1:J:515:ARG:HB3	4:J:959:HOH:O	2.09	0.52
1:2:409:ILE:HG13	1:2:410:HIS:ND1	2.24	0.52
2:B:33:LEU:HD12	2:B:33:LEU:N	2.25	0.52
3:G:137:DMF:H12	2:W:85:ARG:NH2	2.25	0.52
2:I:203:LEU:HB3	2:I:207:SER:OG	2.09	0.52
2:B:47:SER:HB2	4:I:1752:HOH:O	2.10	0.51
2:D:217:ARG:HH11	2:D:223:ARG:HD3	1.75	0.51
1:J:456:GLN:HE22	1:J:465:ARG:HH21	1.58	0.51
2:S:32:ALA:C	2:S:33:LEU:HD12	2.29	0.51
1:C:456:GLN:HE22	1:C:465:ARG:HH21	1.58	0.51
2:I:35:TYR:CE1	2:I:37:GLY:HA3	2.46	0.51
2:I:97:ARG:HB2	4:I:990:HOH:O	2.09	0.51
2:U:85:ARG:HH12	2:U:98:GLN:NE2	2.07	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:85:ARG:NH1	4:W:659:HOH:O	2.41	0.51
2:A:85:ARG:NH1	2:A:98:GLN:NE2	2.58	0.51
2:F:139:TYR:CE1	2:F:149:ASP:HB3	2.46	0.51
2:S:117:PRO:CD	2:1:9:MET:HE1	2.38	0.51
2:B:31:VAL:HG12	2:B:33:LEU:HD12	1.93	0.51
2:F:9:MET:HE1	2:M:116:LYS:HG3	1.92	0.51
2:K:16:ARG:NH2	2:K:114:GLN:O	2.31	0.51
2:K:85:ARG:HH22	3:K:251:DMF:C1	2.23	0.51
2:D:112:THR:HG21	2:Q:116:LYS:HE3	1.91	0.51
2:U:110:ILE:O	2:U:114:GLN:HB2	2.11	0.51
2:1:16:ARG:HB3	2:1:117:PRO:HG3	1.93	0.51
2:A:217:ARG:HH11	2:A:223:ARG:HD3	1.76	0.51
2:I:159:THR:O	2:I:159:THR:CG2	2.56	0.51
2:I:58:ASP:OD1	2:I:219:ARG:NH1	2.44	0.51
2:O:147:ILE:HG12	2:U:50:LEU:HD11	1.91	0.51
1:P:409:ILE:HG13	1:P:410:HIS:ND1	2.26	0.51
1:T:409:ILE:HG13	1:T:410:HIS:ND1	2.26	0.51
2:W:19:LEU:HD23	2:W:19:LEU:O	2.10	0.51
2:O:152:HIS:HB3	2:O:171:TYR:CE2	2.46	0.51
2:Y:217:ARG:HH11	2:Y:223:ARG:HD3	1.76	0.51
2:Y:92:ARG:HD3	2:Y:129:HIS:CE1	2.46	0.51
1:G:472:TYR:CZ	3:G:20:DMF:H22	2.46	0.51
1:N:412:SER:O	1:N:414:PRO:HD3	2.11	0.51
1:P:465:ARG:HD2	4:P:1128:HOH:O	2.10	0.51
2:B:21:ARG:HG3	2:B:22:LYS:N	2.26	0.51
2:M:217:ARG:HH11	2:M:223:ARG:HD3	1.75	0.51
2:F:217:ARG:HH11	2:F:223:ARG:HD3	1.76	0.51
2:K:115:ALA:HB3	4:K:1445:HOH:O	2.11	0.51
1:X:456:GLN:HE22	1:X:465:ARG:HH21	1.59	0.51
2:S:117:PRO:HD3	2:1:9:MET:HE2	1.93	0.50
2:O:217:ARG:HH11	2:O:223:ARG:HD3	1.76	0.50
1:R:409:ILE:HG13	1:R:410:HIS:ND1	2.26	0.50
1:T:472:TYR:CE2	3:T:62:DMF:H13	2.45	0.50
1:Z:409:ILE:HG13	1:Z:410:HIS:ND1	2.26	0.50
2:B:12:ALA:O	2:B:16:ARG:HG3	2.11	0.50
1:G:415:GLN:NE2	4:G:784:HOH:O	2.38	0.50
2:S:18:GLU:OE2	2:S:21:ARG:NH1	2.44	0.50
2:F:105:GLN:HB2	4:F:258:HOH:O	2.11	0.50
2:U:16:ARG:NH2	2:U:114:GLN:O	2.30	0.50
1:Z:366:TYR:CE2	1:Z:374:LEU:HD13	2.46	0.50
2:1:217:ARG:HH11	2:1:223:ARG:HD3	1.75	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:189:ARG:HH12	2:A:203:LEU:N	2.10	0.50
2:F:189:ARG:NH1	2:F:203:LEU:N	2.59	0.50
1:H:366:TYR:CE2	1:H:374:LEU:HD13	2.45	0.50
2:K:49:SER:HB2	2:M:97:ARG:HD2	1.93	0.50
2:Y:85:ARG:NH1	2:Y:98:GLN:NE2	2.59	0.50
2:D:181:LEU:HD23	2:D:233:LEU:HB3	1.94	0.50
1:L:409:ILE:HG13	1:L:410:HIS:ND1	2.27	0.50
1:N:409:ILE:HG13	1:N:410:HIS:ND1	2.26	0.50
2:U:152:HIS:HB3	2:U:171:TYR:CE2	2.46	0.50
1:G:409:ILE:HG13	1:G:410:HIS:ND1	2.27	0.50
1:L:339:ASP:HB2	3:L:138:DMF:H12	1.94	0.50
2:M:152:HIS:HB3	2:M:171:TYR:CE2	2.46	0.50
1:J:412:SER:O	1:J:414:PRO:HD3	2.12	0.50
2:D:152:HIS:HB3	2:D:171:TYR:CE2	2.47	0.50
2:I:55:GLU:HB2	2:I:222:PHE:CG	2.47	0.50
2:S:152:HIS:HB3	2:S:171:TYR:CE2	2.47	0.50
2:I:85:ARG:NH1	2:I:98:GLN:NE2	2.60	0.49
2:B:32:ALA:HB3	2:B:154:VAL:HG23	1.92	0.49
1:E:391:LEU:HD21	1:L:398:LEU:HD11	1.93	0.49
2:F:16:ARG:HB3	2:F:117:PRO:HG3	1.94	0.49
2:K:116:LYS:HG2	2:K:117:PRO:HD2	1.93	0.49
2:F:85:ARG:NH1	2:F:98:GLN:NE2	2.60	0.49
2:K:217:ARG:HH11	2:K:223:ARG:HD3	1.76	0.49
1:Z:456:GLN:HE22	1:Z:465:ARG:HH21	1.60	0.49
2:F:150:GLU:HG3	2:F:154:VAL:HG22	1.93	0.49
1:P:456:GLN:HE22	1:P:465:ARG:HH21	1.59	0.49
2:S:189:ARG:HH12	2:S:203:LEU:N	2.11	0.49
2:F:97:ARG:NH1	4:F:866:HOH:O	2.45	0.49
1:R:412:SER:O	1:R:414:PRO:HD3	2.12	0.49
1:X:409:ILE:HG13	1:X:410:HIS:ND1	2.27	0.49
1:T:456:GLN:HE22	1:T:465:ARG:HH21	1.59	0.49
1:C:409:ILE:HG13	1:C:410:HIS:ND1	2.27	0.49
2:I:11:GLN:CG	2:I:14:ARG:HH12	2.09	0.49
2:I:35:TYR:CE2	2:I:38:GLY:O	2.66	0.49
2:K:152:HIS:HB3	2:K:171:TYR:CE2	2.47	0.49
1:J:391:LEU:HD21	1:T:398:LEU:HD11	1.95	0.49
2:Y:189:ARG:NH1	2:Y:203:LEU:N	2.59	0.49
1:E:520:SER:HB3	4:E:1913:HOH:O	2.12	0.49
2:I:182:ARG:NH2	4:I:719:HOH:O	2.45	0.49
1:L:456:GLN:HE22	1:L:465:ARG:HH21	1.60	0.49
1:N:456:GLN:HE22	1:N:465:ARG:HH21	1.61	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:U:18:GLU:HA	2:U:21:ARG:NH2	2.27	0.49
1:Z:412:SER:O	1:Z:414:PRO:HD3	2.13	0.49
2:B:35:TYR:CE1	2:B:177:LEU:CD1	2.96	0.49
1:C:348:THR:HA	4:C:1685:HOH:O	2.13	0.49
2:F:149:ASP:O	2:F:149:ASP:OD1	2.30	0.49
2:S:178:THR:HG23	2:S:179:ASP:N	2.27	0.49
1:Z:444:LEU:HB2	4:Z:692:HOH:O	2.12	0.49
2:B:189:ARG:HE	2:B:189:ARG:HA	1.75	0.49
1:X:366:TYR:CE2	1:X:374:LEU:HD13	2.47	0.49
2:1:152:HIS:HB3	2:1:171:TYR:CE2	2.48	0.49
2:A:97:ARG:HD2	2:O:49:SER:HB2	1.95	0.49
1:E:412:SER:O	1:E:414:PRO:HD3	2.13	0.49
2:I:11:GLN:CG	2:I:14:ARG:CZ	2.90	0.49
2:U:9:MET:HE2	2:U:13:MET:CE	2.42	0.49
1:V:345:ILE:O	3:V:136:DMF:H21	2.12	0.49
1:Z:429:TRP:CH2	3:Z:105:DMF:H13	2.48	0.49
2:1:102:VAL:HG13	3:1:249:DMF:H12	1.94	0.48
1:J:366:TYR:CE2	1:J:374:LEU:HD13	2.48	0.48
2:M:85:ARG:HB3	4:M:781:HOH:O	2.12	0.48
1:R:456:GLN:HE22	1:R:465:ARG:HH21	1.61	0.48
1:V:409:ILE:HG13	1:V:410:HIS:ND1	2.28	0.48
2:Q:9:MET:N	2:Y:15:GLU:OE1	2.46	0.48
2:B:67:LYS:HE3	2:B:69:ASN:OD1	2.14	0.48
2:F:9:MET:CE	2:M:116:LYS:HA	2.43	0.48
2:I:16:ARG:HB3	2:I:117:PRO:HG3	1.96	0.48
1:J:409:ILE:HG13	1:J:410:HIS:ND1	2.28	0.48
1:N:366:TYR:CE2	1:N:374:LEU:HD13	2.48	0.48
2:F:152:HIS:HB3	2:F:171:TYR:CE2	2.47	0.48
2:B:166:ALA:CB	2:B:187:ALA:CA	2.90	0.48
1:E:409:ILE:HG13	1:E:410:HIS:ND1	2.28	0.48
1:G:412:SER:O	1:G:414:PRO:HD3	2.13	0.48
2:Q:217:ARG:NH1	2:Q:223:ARG:HD3	2.29	0.48
2:B:110:ILE:O	2:B:114:GLN:HB2	2.13	0.48
2:D:19:LEU:C	2:D:19:LEU:HD23	2.34	0.48
1:H:409:ILE:HG13	1:H:410:HIS:ND1	2.28	0.48
1:E:444:LEU:HD21	1:L:325:MET:SD	2.54	0.48
2:O:27:ALA:HB1	4:O:1192:HOH:O	2.14	0.48
1:P:366:TYR:CE2	1:P:374:LEU:HD13	2.49	0.48
2:U:16:ARG:HB3	2:U:117:PRO:HG2	1.95	0.48
2:B:161:GLU:N	2:B:162:PRO:HD2	2.29	0.48
1:C:412:SER:O	1:C:414:PRO:HD3	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:181:LEU:HD23	2:O:233:LEU:HB3	1.95	0.48
2:U:19:LEU:HD23	2:U:19:LEU:C	2.33	0.48
1:2:366:TYR:CE2	1:2:374:LEU:HD13	2.48	0.48
2:B:94:VAL:HA	2:B:98:GLN:OE1	2.12	0.48
2:D:35:TYR:CZ	2:D:37:GLY:HA3	2.47	0.48
1:L:366:TYR:CE2	1:L:374:LEU:HD13	2.49	0.48
1:N:465:ARG:NH1	4:N:611:HOH:O	2.47	0.48
2:Q:74:LEU:HD13	2:Q:122:LEU:HD11	1.95	0.48
2:U:16:ARG:HB3	2:U:117:PRO:CG	2.44	0.48
1:V:357:ARG:HA	3:V:117:DMF:HC	1.95	0.48
2:Y:185:VAL:O	2:Y:189:ARG:HG3	2.14	0.48
1:E:456:GLN:HE22	1:E:465:ARG:HH21	1.60	0.48
2:I:12:ALA:O	2:I:16:ARG:HG3	2.14	0.48
2:B:49:SER:OG	2:I:97:ARG:HG3	2.13	0.48
1:P:412:SER:O	1:P:414:PRO:HD3	2.14	0.48
2:S:41:PHE:HB3	2:S:53:ILE:HD13	1.96	0.48
2:B:129:HIS:HD2	4:B:1916:HOH:O	1.97	0.47
2:B:64:ALA:HB2	2:B:122:LEU:HD22	1.83	0.47
2:W:18:GLU:CD	2:W:21:ARG:NH1	2.67	0.47
1:L:412:SER:O	1:L:414:PRO:HD3	2.12	0.47
1:V:412:SER:O	1:V:414:PRO:HD3	2.14	0.47
2:Y:203:LEU:CD1	2:Y:203:LEU:N	2.77	0.47
1:C:375:THR:HG21	2:I:92:ARG:HB3	1.96	0.47
2:D:217:ARG:NH1	2:D:223:ARG:HD3	2.30	0.47
2:Q:51:GLN:HB2	4:Q:255:HOH:O	2.14	0.47
2:U:9:MET:HE2	2:U:13:MET:HE2	1.95	0.47
1:2:412:SER:HB2	4:2:543:HOH:O	2.14	0.47
1:T:412:SER:O	1:T:414:PRO:HD3	2.14	0.47
2:A:205:VAL:HG22	2:A:230:LEU:HD23	1.97	0.47
2:B:60:VAL:HG11	2:B:99:LEU:HD12	1.95	0.47
2:I:152:HIS:CG	2:I:171:TYR:CE2	3.03	0.47
2:O:21:ARG:NH2	4:O:680:HOH:O	2.47	0.47
2:Y:97:ARG:CZ	4:Y:849:HOH:O	2.61	0.47
1:H:456:GLN:HE22	1:H:465:ARG:HH21	1.61	0.47
1:E:398:LEU:HD11	1:R:391:LEU:HD21	1.95	0.47
2:U:233:LEU:CD1	2:U:233:LEU:N	2.77	0.47
2:B:141:ILE:N	2:B:141:ILE:HD12	2.30	0.47
2:F:12:ALA:O	2:F:16:ARG:HG3	2.14	0.47
1:H:325:MET:SD	1:P:444:LEU:HD21	2.55	0.47
2:Y:19:LEU:HD23	2:Y:19:LEU:C	2.35	0.47
1:2:412:SER:O	1:2:414:PRO:HD3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:114:GLN:NE2	4:M:1233:HOH:O	2.48	0.47
2:Q:11:GLN:OE1	2:Q:15:GLU:HG3	2.14	0.47
2:W:135:ARG:NE	4:W:2032:HOH:O	2.48	0.47
2:Y:18:GLU:O	2:Y:22:LYS:HG3	2.13	0.47
2:A:18:GLU:CD	2:A:21:ARG:NH1	2.64	0.47
2:A:217:ARG:NH1	2:A:223:ARG:HD3	2.30	0.47
2:B:42:VAL:HG23	2:B:210:VAL:HG22	1.96	0.47
3:E:113:DMF:H22	1:R:429:TRP:CZ2	2.50	0.47
1:T:366:TYR:CE2	1:T:374:LEU:HD13	2.49	0.47
2:A:73:ASN:OD1	2:B:105:GLN:NE2	2.48	0.47
1:H:412:SER:O	1:H:414:PRO:HD3	2.15	0.47
2:M:217:ARG:NH1	2:M:223:ARG:HD3	2.29	0.47
2:A:85:ARG:NH2	3:A:249:DMF:H22	2.30	0.46
2:F:32:ALA:C	2:F:33:LEU:HD12	2.36	0.46
2:I:56:LEU:HG	2:I:62:PHE:HB2	1.96	0.46
2:B:212:VAL:HG23	2:B:223:ARG:HG3	1.97	0.46
2:B:210:VAL:HG12	2:B:225:ILE:HG12	1.97	0.46
2:D:18:GLU:CD	2:D:21:ARG:NH1	2.68	0.46
1:J:456:GLN:NE2	1:J:465:ARG:HH21	2.13	0.46
3:P:133:DMF:H22	2:O:91:ARG:NH1	2.31	0.46
2:W:217:ARG:NH1	2:W:223:ARG:HD3	2.29	0.46
1:X:412:SER:O	1:X:414:PRO:HD3	2.15	0.46
2:1:217:ARG:NH1	2:1:223:ARG:HD3	2.30	0.46
2:1:106:THR:HG21	3:1:249:DMF:HC	1.97	0.46
2:Q:179:ASP:O	2:Q:183:ILE:HG13	2.15	0.46
1:T:377:ALA:CB	3:T:134:DMF:H13	2.45	0.46
2:W:161:GLU:CB	2:W:162:PRO:HD3	2.45	0.46
2:B:74:LEU:CD1	2:B:122:LEU:HD11	2.46	0.46
1:E:520:SER:CB	4:E:1913:HOH:O	2.64	0.46
2:O:217:ARG:NH1	2:O:223:ARG:HD3	2.31	0.46
1:P:456:GLN:NE2	1:P:465:ARG:HH21	2.14	0.46
2:Q:181:LEU:HD21	2:Q:234:LEU:HD13	1.96	0.46
2:U:217:ARG:NH1	2:U:223:ARG:HD3	2.29	0.46
2:B:55:GLU:HB3	2:B:222:PHE:CB	2.45	0.46
2:M:12:ALA:O	2:M:16:ARG:HG3	2.15	0.46
2:K:76:ARG:HD3	4:K:255:HOH:O	2.15	0.46
2:Q:27:ALA:HB1	4:Q:5:HOH:O	2.15	0.46
2:Y:217:ARG:NH1	2:Y:223:ARG:HD3	2.30	0.46
1:G:456:GLN:HE22	1:G:465:ARG:HH21	1.63	0.46
2:O:16:ARG:HB3	2:O:117:PRO:HG3	1.98	0.46
1:X:456:GLN:NE2	1:X:465:ARG:HH21	2.12	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:366:TYR:CE2	1:G:374:LEU:HD13	2.50	0.46
2:I:39:VAL:HG21	2:I:125:ALA:HB1	1.98	0.46
2:Q:135:ARG:NH2	2:Q:173:GLU:OE1	2.49	0.46
1:C:401:LEU:HA	1:C:402:PRO:HD3	1.85	0.46
1:C:456:GLN:NE2	1:C:465:ARG:HH21	2.14	0.46
2:K:97:ARG:NH1	4:K:1647:HOH:O	2.49	0.46
2:B:90:ASP:OD1	2:B:90:ASP:O	2.34	0.45
1:E:444:LEU:HB2	4:E:601:HOH:O	2.15	0.45
2:I:99:LEU:HA	2:I:102:VAL:HG12	1.98	0.45
2:F:9:MET:HE1	2:M:117:PRO:HD3	1.97	0.45
1:C:479:SER:HB2	1:E:479:SER:HB2	1.98	0.45
1:L:482:GLY:HA3	4:L:582:HOH:O	2.15	0.45
2:S:30:VAL:HG13	2:S:43:ALA:HB2	1.98	0.45
2:B:16:ARG:NH2	2:B:114:GLN:O	2.30	0.45
1:J:515:ARG:NH1	4:J:1880:HOH:O	2.48	0.45
2:S:85:ARG:NH1	4:S:1099:HOH:O	2.44	0.45
2:W:31:VAL:HG12	2:W:155:VAL:HG22	1.97	0.45
2:D:9:MET:N	2:Q:15:GLU:OE1	2.50	0.45
2:F:54:SER:CB	2:F:75:ARG:HD2	2.47	0.45
2:Y:9:MET:SD	2:Y:9:MET:O	2.74	0.45
2:F:217:ARG:NH1	2:F:223:ARG:HD3	2.30	0.45
2:I:152:HIS:HB3	2:I:171:TYR:CZ	2.48	0.45
2:K:15:GLU:HB3	2:M:9:MET:N	2.31	0.45
2:W:97:ARG:NH1	4:W:1712:HOH:O	2.50	0.45
2:Q:97:ARG:CD	2:Y:49:SER:HB2	2.46	0.45
2:B:9:MET:HE1	2:B:13:MET:CE	2.23	0.45
2:D:35:TYR:CD1	2:D:37:GLY:N	2.80	0.45
2:F:112:THR:HG21	2:M:116:LYS:HE3	1.99	0.45
1:L:416:SER:HA	4:L:2014:HOH:O	2.16	0.45
2:Y:189:ARG:HH11	2:Y:203:LEU:HD12	1.81	0.45
2:B:141:ILE:HG13	2:B:147:ILE:CD1	2.46	0.45
2:K:217:ARG:NH1	2:K:223:ARG:HD3	2.31	0.45
1:N:473:ASP:OD1	1:N:521:ARG:NH1	2.37	0.45
2:O:185:VAL:O	2:O:189:ARG:HG2	2.16	0.45
2:Q:54:SER:CB	2:Q:75:ARG:HD2	2.46	0.45
1:T:456:GLN:NE2	1:T:465:ARG:HH21	2.14	0.45
2:W:181:LEU:HD13	2:W:233:LEU:HB3	1.98	0.45
2:B:155:VAL:HG22	2:B:160:THR:HB	1.98	0.45
2:B:57:TYR:CZ	2:B:91:ARG:NH1	2.84	0.45
1:E:401:LEU:HA	1:E:402:PRO:HD3	1.84	0.45
2:M:151:PRO:HD2	4:M:1408:HOH:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:30:VAL:HG13	2:O:43:ALA:HB2	1.99	0.45
2:Y:16:ARG:HB3	2:Y:117:PRO:HG3	1.99	0.45
2:A:41:PHE:HB3	2:A:53:ILE:HD13	1.99	0.45
2:B:9:MET:CE	2:B:13:MET:HE1	2.40	0.45
2:D:150:GLU:HA	2:D:151:PRO:HD3	1.82	0.45
1:L:456:GLN:NE2	1:L:465:ARG:HH21	2.15	0.45
2:Q:11:GLN:CA	2:Q:11:GLN:NE2	2.80	0.45
1:Z:456:GLN:NE2	1:Z:465:ARG:HH21	2.15	0.45
2:A:230:LEU:O	2:A:231:GLN:C	2.55	0.45
2:A:45:ASN:HA	2:A:46:PRO:HD3	1.83	0.45
1:C:366:TYR:CE2	1:C:374:LEU:HD13	2.52	0.45
1:P:471:LEU:HA	1:P:471:LEU:HD12	1.87	0.45
2:S:182:ARG:NH1	4:S:1950:HOH:O	2.49	0.45
2:A:181:LEU:HD23	2:A:233:LEU:HB3	2.00	0.44
2:B:116:LYS:HB2	2:I:13:MET:HE3	1.98	0.44
2:B:99:LEU:HA	2:B:99:LEU:HD23	1.86	0.44
2:F:139:TYR:CD1	2:F:149:ASP:HB3	2.53	0.44
2:F:229:ALA:O	2:F:232:ALA:HB3	2.17	0.44
2:1:30:VAL:HG13	2:1:43:ALA:HB2	2.00	0.44
2:B:32:ALA:HA	2:B:40:LEU:O	2.17	0.44
1:C:473:ASP:OD2	1:R:452:LYS:NZ	2.37	0.44
1:E:375:THR:HG21	2:K:92:ARG:HB3	2.00	0.44
2:O:189:ARG:CD	2:O:203:LEU:HD12	2.47	0.44
2:D:32:ALA:C	2:D:33:LEU:HD12	2.37	0.44
1:H:456:GLN:NE2	1:H:465:ARG:HH21	2.15	0.44
1:X:471:LEU:HA	1:X:471:LEU:HD12	1.87	0.44
2:Y:188:LEU:HA	2:Y:188:LEU:HD12	1.89	0.44
2:A:32:ALA:C	2:A:33:LEU:HD12	2.38	0.44
1:J:471:LEU:HD12	1:J:471:LEU:HA	1.84	0.44
1:L:379:LYS:HZ3	3:L:138:DMF:HC	1.81	0.44
2:M:150:GLU:HA	2:M:151:PRO:HD3	1.84	0.44
1:R:509:ARG:O	1:R:513:LEU:HD13	2.18	0.44
1:V:456:GLN:HE22	1:V:465:ARG:HH21	1.66	0.44
2:W:181:LEU:HD23	2:W:185:VAL:HG23	1.99	0.44
1:X:396:GLN:HB3	1:X:396:GLN:HE21	1.60	0.44
1:2:472:TYR:CE1	3:2:99:DMF:H13	2.53	0.44
2:B:52:LYS:O	2:B:53:ILE:HD13	2.18	0.44
2:D:107:LEU:HA	2:D:107:LEU:HD23	1.88	0.44
1:N:429:TRP:CH2	3:N:21:DMF:H13	2.52	0.44
1:N:456:GLN:NE2	1:N:465:ARG:HH21	2.16	0.44
1:V:429:TRP:CE2	3:V:121:DMF:H22	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:173:GLU:O	2:Y:174:ASN:HB2	2.17	0.44
2:A:168:LYS:HB2	2:A:168:LYS:HE3	1.79	0.44
2:A:30:VAL:HG13	2:A:43:ALA:HB2	1.99	0.44
1:H:363:LEU:HD12	1:H:363:LEU:HA	1.88	0.44
2:S:168:LYS:HE3	2:S:168:LYS:HB2	1.78	0.44
2:S:102:VAL:HG13	3:S:249:DMF:H12	2.00	0.44
2:U:189:ARG:HG2	2:U:203:LEU:HD12	1.98	0.44
2:W:150:GLU:HA	2:W:151:PRO:HD3	1.83	0.44
2:B:18:GLU:CD	2:B:21:ARG:HD3	2.38	0.44
1:C:306:LEU:HD12	1:C:306:LEU:O	2.18	0.44
2:D:168:LYS:HB2	2:D:168:LYS:HE3	1.77	0.44
2:K:116:LYS:CG	2:K:117:PRO:HD2	2.47	0.44
1:L:379:LYS:NZ	3:L:138:DMF:HC	2.32	0.44
2:O:85:ARG:HH12	2:O:98:GLN:HE21	1.63	0.44
1:R:432:GLU:HB2	4:R:1661:HOH:O	2.17	0.44
2:W:189:ARG:NH2	4:W:1576:HOH:O	2.50	0.44
2:W:41:PHE:HB3	2:W:53:ILE:HD13	1.99	0.44
1:N:388:ARG:NE	4:N:1663:HOH:O	2.47	0.44
2:O:168:LYS:HB2	2:O:168:LYS:HE3	1.78	0.44
2:S:116:LYS:HE3	2:I:112:THR:HG21	2.00	0.44
2:D:116:LYS:HE3	2:K:112:THR:HG21	2.00	0.43
2:U:147:ILE:HG21	2:I:68:PHE:CD2	2.53	0.43
2:F:30:VAL:HG13	2:F:43:ALA:HB2	2.00	0.43
1:G:456:GLN:NE2	1:G:465:ARG:HH21	2.16	0.43
1:R:366:TYR:OH	2:D:93:ASP:HB3	2.19	0.43
2:B:56:LEU:HD13	2:B:99:LEU:HD13	1.99	0.43
1:E:456:GLN:NE2	1:E:465:ARG:HH21	2.16	0.43
2:F:9:MET:HE1	2:M:117:PRO:CD	2.48	0.43
2:I:41:PHE:HB3	2:I:53:ILE:HD13	2.00	0.43
2:U:181:LEU:CD2	2:U:233:LEU:HB3	2.49	0.43
2:Y:228:SER:O	2:Y:229:ALA:C	2.56	0.43
2:I:54:SER:CB	2:I:75:ARG:HD2	2.48	0.43
2:A:9:MET:O	2:A:13:MET:HG2	2.19	0.43
1:G:363:LEU:HA	1:G:363:LEU:HD12	1.88	0.43
1:L:410:HIS:HD2	4:M:1361:HOH:O	2.00	0.43
2:M:32:ALA:C	2:M:33:LEU:HD12	2.38	0.43
2:O:41:PHE:HB3	2:O:53:ILE:HD13	2.00	0.43
2:A:54:SER:CB	2:A:75:ARG:HD2	2.48	0.43
1:C:471:LEU:HA	1:C:471:LEU:HD12	1.83	0.43
2:D:230:LEU:O	2:D:234:LEU:HD13	2.19	0.43
1:R:456:GLN:NE2	1:R:465:ARG:HH21	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:54:SER:CB	2:S:75:ARG:HD2	2.48	0.43
1:N:375:THR:HG21	2:F:92:ARG:HB3	2.00	0.43
1:T:444:LEU:HD21	1:2:325:MET:SD	2.58	0.43
2:U:41:PHE:HB3	2:U:53:ILE:HD13	2.01	0.43
2:U:54:SER:CB	2:U:75:ARG:HD2	2.49	0.43
2:1:151:PRO:HD2	4:1:393:HOH:O	2.19	0.43
1:2:306:LEU:HD12	1:2:306:LEU:O	2.19	0.43
2:B:59:ARG:HD2	2:B:127:VAL:CG1	2.45	0.43
2:O:189:ARG:HD2	2:O:203:LEU:CD1	2.48	0.43
2:Y:41:PHE:HB3	2:Y:53:ILE:HD13	2.01	0.43
2:B:64:ALA:HB1	2:B:122:LEU:CD2	2.43	0.43
2:1:41:PHE:HB3	2:1:53:ILE:HD13	2.01	0.43
1:2:401:LEU:HA	1:2:402:PRO:HD3	1.86	0.43
2:B:207:SER:O	2:B:208:LEU:HG	2.19	0.43
1:G:471:LEU:HA	1:G:471:LEU:HD12	1.91	0.43
1:J:306:LEU:C	1:J:306:LEU:HD12	2.40	0.43
2:U:147:ILE:HG12	2:1:50:LEU:HD11	2.01	0.43
2:B:40:LEU:CD1	2:B:212:VAL:HG13	2.48	0.43
2:B:217:ARG:HG3	2:B:223:ARG:NH2	2.14	0.43
1:P:377:ALA:HB1	3:P:107:DMF:C	2.49	0.43
2:S:33:LEU:N	2:S:33:LEU:HD12	2.34	0.43
1:V:363:LEU:HD12	1:V:363:LEU:HA	1.87	0.43
1:E:509:ARG:NH2	4:E:1830:HOH:O	2.48	0.42
2:U:225:ILE:HG22	2:U:230:LEU:HA	2.01	0.42
2:D:33:LEU:HD12	2:D:33:LEU:N	2.33	0.42
2:D:35:TYR:CE1	2:D:37:GLY:N	2.88	0.42
1:E:456:GLN:HG3	4:E:2203:HOH:O	2.19	0.42
2:O:13:MET:HG3	2:U:19:LEU:HD11	2.01	0.42
2:D:85:ARG:HH22	3:Q:251:DMF:C2	2.31	0.42
2:U:9:MET:CE	2:U:13:MET:HE3	2.47	0.42
2:D:129:HIS:HE1	4:D:1211:HOH:O	2.01	0.42
2:D:41:PHE:HB3	2:D:53:ILE:HD13	2.01	0.42
2:D:54:SER:CB	2:D:75:ARG:HD2	2.49	0.42
1:J:368:LYS:HB3	2:I:79:ILE:HD13	2.00	0.42
2:K:54:SER:CB	2:K:75:ARG:HD2	2.49	0.42
2:K:225:ILE:HG22	2:K:230:LEU:HA	2.01	0.42
1:L:375:THR:HG21	2:M:92:ARG:HB3	2.01	0.42
2:Y:128:ALA:HB2	2:Y:134:LYS:HB3	2.01	0.42
2:Y:32:ALA:C	2:Y:33:LEU:HD12	2.39	0.42
2:B:224:ARG:HG3	2:B:224:ARG:O	2.20	0.42
2:Y:18:GLU:CD	2:Y:21:ARG:HH12	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:150:GLU:HA	2:B:151:PRO:HD3	1.82	0.42
1:E:496:ILE:HD12	4:E:1830:HOH:O	2.20	0.42
1:G:401:LEU:HA	1:G:402:PRO:HD3	1.85	0.42
1:P:381:ASN:HB2	3:P:107:DMF:H12	2.02	0.42
2:Q:41:PHE:HB3	2:Q:53:ILE:HD13	1.99	0.42
1:V:471:LEU:HD12	1:V:471:LEU:HA	1.88	0.42
2:B:135:ARG:NH2	2:B:173:GLU:OE2	2.53	0.42
2:B:161:GLU:OE1	2:B:161:GLU:HA	2.19	0.42
2:B:59:ARG:NH2	2:B:130:TYR:HB2	2.34	0.42
2:U:168:LYS:HB2	2:U:168:LYS:HE3	1.78	0.42
2:W:9:MET:N	2:W:9:MET:SD	2.93	0.42
2:B:110:ILE:O	2:B:114:GLN:CB	2.68	0.42
2:B:62:PHE:CE1	2:B:122:LEU:HD22	2.55	0.42
1:E:380:ILE:HG21	3:E:104:DMF:H12	2.01	0.42
2:O:54:SER:CB	2:O:75:ARG:HD2	2.50	0.42
1:R:306:LEU:C	1:R:306:LEU:HD12	2.39	0.42
1:V:388:ARG:NE	4:V:1388:HOH:O	2.40	0.42
2:B:40:LEU:HD12	2:B:212:VAL:HG13	2.01	0.42
2:M:30:VAL:HG13	2:M:43:ALA:HB2	2.01	0.42
2:M:33:LEU:HD12	2:M:33:LEU:N	2.35	0.42
2:M:54:SER:CB	2:M:75:ARG:HD2	2.49	0.42
2:S:45:ASN:HA	2:S:46:PRO:HD3	1.82	0.42
2:U:170:SER:OG	2:U:183:ILE:HG23	2.20	0.42
2:Y:54:SER:CB	2:Y:75:ARG:HD2	2.49	0.42
1:2:306:LEU:HD12	1:2:306:LEU:C	2.40	0.42
2:A:115:ALA:HB3	2:B:112:THR:HG21	1.83	0.42
2:F:150:GLU:HA	2:F:151:PRO:HD3	1.83	0.41
2:K:102:VAL:HG13	3:K:249:DMF:H12	2.02	0.41
2:M:53:ILE:O	2:M:224:ARG:NH2	2.50	0.41
1:V:515:ARG:HD2	4:V:2036:HOH:O	2.21	0.41
2:B:230:LEU:CD2	2:B:230:LEU:C	2.88	0.41
2:K:150:GLU:HA	2:K:151:PRO:HD3	1.83	0.41
1:R:306:LEU:O	1:R:306:LEU:HD12	2.20	0.41
2:W:167:LEU:HD12	2:W:167:LEU:HA	1.80	0.41
2:W:32:ALA:C	2:W:33:LEU:HD12	2.40	0.41
2:W:54:SER:CB	2:W:75:ARG:HD2	2.50	0.41
1:2:429:TRP:CH2	3:2:145:DMF:H23	2.55	0.41
2:I:30:VAL:HG13	2:I:43:ALA:HB2	2.02	0.41
2:K:41:PHE:HB3	2:K:53:ILE:HD13	2.01	0.41
2:O:150:GLU:HA	2:O:151:PRO:HD3	1.83	0.41
2:O:217:ARG:HA	2:O:218:PRO:HD3	1.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:U:106:THR:O	2:U:110:ILE:HG13	2.20	0.41
2:W:19:LEU:CD2	2:W:19:LEU:C	2.86	0.41
2:W:45:ASN:HA	2:W:46:PRO:HD3	1.84	0.41
1:Z:357:ARG:HD3	4:Z:1337:HOH:O	2.19	0.41
2:1:167:LEU:HG	2:1:187:ALA:HB1	2.01	0.41
2:B:19:LEU:CD2	2:B:19:LEU:C	2.86	0.41
1:X:391:LEU:CD2	1:Z:398:LEU:HD11	2.48	0.41
2:B:225:ILE:HG13	2:B:230:LEU:HG	2.02	0.41
2:S:150:GLU:HA	2:S:151:PRO:HD3	1.84	0.41
1:N:306:LEU:C	1:N:306:LEU:HD12	2.41	0.41
2:Q:16:ARG:NE	2:Q:111:PHE:O	2.53	0.41
2:U:30:VAL:HG13	2:U:43:ALA:HB2	2.03	0.41
2:W:213:LEU:HD23	2:W:213:LEU:HA	1.93	0.41
1:2:396:GLN:HB3	1:2:396:GLN:HE21	1.60	0.41
2:D:49:SER:HB2	2:K:97:ARG:HD2	2.02	0.41
2:Q:168:LYS:HE3	2:Q:168:LYS:HB2	1.80	0.41
1:Z:429:TRP:CZ2	3:Z:105:DMF:H22	2.56	0.41
2:A:19:LEU:O	2:A:19:LEU:HD23	2.19	0.41
2:D:116:LYS:CG	2:D:117:PRO:HD2	2.50	0.41
2:F:41:PHE:HB3	2:F:53:ILE:HD13	2.03	0.41
2:U:9:MET:CE	2:U:13:MET:HE2	2.50	0.41
2:1:38:GLY:HA3	2:1:213:LEU:O	2.21	0.41
2:B:100:ALA:HB1	2:B:147:ILE:HD11	2.02	0.41
1:H:415:GLN:HA	1:H:415:GLN:OE1	2.21	0.41
2:O:11:GLN:HA	2:O:14:ARG:HB3	2.03	0.41
1:V:456:GLN:NE2	1:V:465:ARG:HH21	2.18	0.41
2:I:32:ALA:HA	2:I:40:LEU:O	2.21	0.41
1:Z:363:LEU:HD12	1:Z:363:LEU:HA	1.85	0.41
2:A:234:LEU:HD12	2:A:234:LEU:HA	1.90	0.41
2:B:217:ARG:CG	2:B:217:ARG:HH11	2.03	0.41
2:B:70:GLU:HG2	2:B:118:TYR:CE1	2.56	0.41
1:H:517:ILE:O	1:H:521:ARG:HG3	2.21	0.41
2:I:54:SER:CB	2:I:75:ARG:HD2	2.51	0.41
1:P:513:LEU:HA	1:P:513:LEU:HD12	1.90	0.41
1:R:401:LEU:HA	1:R:402:PRO:HD3	1.83	0.41
1:C:476:ASP:HB3	1:R:451:LYS:HZ1	1.86	0.41
2:O:9:MET:HE1	2:U:115:ALA:O	2.20	0.41
2:1:24:ILE:HG22	2:1:157:GLY:HA2	2.03	0.40
2:B:133:THR:HG22	2:B:133:THR:O	2.21	0.40
2:B:53:ILE:HB	4:B:1703:HOH:O	2.21	0.40
2:D:52:LYS:HB3	2:D:52:LYS:HE2	1.90	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:217:ARG:HA	2:Y:218:PRO:HD3	1.89	0.40
2:Q:147:ILE:HG12	2:Y:50:LEU:HD11	2.02	0.40
2:B:217:ARG:HA	4:B:751:HOH:O	2.20	0.40
2:F:9:MET:HE1	2:M:116:LYS:HA	2.02	0.40
2:O:35:TYR:HB2	2:O:175:ALA:O	2.21	0.40
1:T:472:TYR:OH	3:T:62:DMF:H13	2.22	0.40
2:U:226:THR:HG22	4:U:252:HOH:O	2.21	0.40
2:B:47:SER:HB2	2:I:149:ASP:CG	2.39	0.40
2:M:189:ARG:HH12	2:M:203:LEU:N	2.20	0.40
2:Q:30:VAL:HG13	2:Q:43:ALA:HB2	2.02	0.40
2:Y:129:HIS:O	2:Y:132:GLU:HG2	2.21	0.40
2:W:16:ARG:NH1	2:Y:9:MET:HG3	2.36	0.40
2:Y:9:MET:SD	2:Y:9:MET:C	2.99	0.40
2:F:38:GLY:HA3	2:F:213:LEU:O	2.21	0.40
1:R:363:LEU:HA	1:R:363:LEU:HD12	1.88	0.40
1:X:465:ARG:NH1	4:X:1509:HOH:O	2.54	0.40
1:Z:465:ARG:NH1	4:Z:1776:HOH:O	2.53	0.40
2:B:104:ALA:HB1	2:B:145:GLY:O	2.21	0.40
2:B:116:LYS:HE3	2:I:112:THR:HG21	2.03	0.40
2:B:81:PHE:CE2	2:B:85:ARG:HG3	2.57	0.40
2:K:101:ASN:HB3	3:K:251:DMF:C2	2.51	0.40
1:N:332:ARG:HB3	4:N:1560:HOH:O	2.20	0.40
1:T:306:LEU:HD12	1:T:306:LEU:O	2.22	0.40
2:U:24:ILE:CD1	2:U:143:TYR:HD2	2.34	0.40
4:T:1393:HOH:O	1:X:451:LYS:HE3	2.20	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	2	220/240 (92%)	218 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	220/240 (92%)	220 (100%)	0	0	100	100
1	E	221/240 (92%)	219 (99%)	2 (1%)	0	100	100
1	G	220/240 (92%)	218 (99%)	2 (1%)	0	100	100
1	H	221/240 (92%)	219 (99%)	2 (1%)	0	100	100
1	J	220/240 (92%)	219 (100%)	1 (0%)	0	100	100
1	L	220/240 (92%)	218 (99%)	2 (1%)	0	100	100
1	N	221/240 (92%)	218 (99%)	3 (1%)	0	100	100
1	P	220/240 (92%)	218 (99%)	2 (1%)	0	100	100
1	R	220/240 (92%)	218 (99%)	2 (1%)	0	100	100
1	T	221/240 (92%)	219 (99%)	2 (1%)	0	100	100
1	V	224/240 (93%)	222 (99%)	2 (1%)	0	100	100
1	X	222/240 (92%)	220 (99%)	2 (1%)	0	100	100
1	Z	222/240 (92%)	221 (100%)	1 (0%)	0	100	100
2	1	210/240 (88%)	206 (98%)	4 (2%)	0	100	100
2	A	210/240 (88%)	206 (98%)	4 (2%)	0	100	100
2	B	210/240 (88%)	201 (96%)	9 (4%)	0	100	100
2	D	209/240 (87%)	205 (98%)	4 (2%)	0	100	100
2	F	210/240 (88%)	206 (98%)	4 (2%)	0	100	100
2	I	210/240 (88%)	206 (98%)	4 (2%)	0	100	100
2	K	210/240 (88%)	206 (98%)	4 (2%)	0	100	100
2	M	210/240 (88%)	206 (98%)	4 (2%)	0	100	100
2	O	210/240 (88%)	205 (98%)	5 (2%)	0	100	100
2	Q	210/240 (88%)	206 (98%)	4 (2%)	0	100	100
2	S	210/240 (88%)	204 (97%)	6 (3%)	0	100	100
2	U	210/240 (88%)	205 (98%)	5 (2%)	0	100	100
2	W	210/240 (88%)	207 (99%)	3 (1%)	0	100	100
2	Y	210/240 (88%)	205 (98%)	5 (2%)	0	100	100
All	All	6031/6720 (90%)	5941 (98%)	90 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	2	165/178 (93%)	160 (97%)	5 (3%)	41	68
1	C	165/178 (93%)	159 (96%)	6 (4%)	35	61
1	E	165/178 (93%)	160 (97%)	5 (3%)	41	68
1	G	165/178 (93%)	158 (96%)	7 (4%)	30	54
1	H	165/178 (93%)	159 (96%)	6 (4%)	35	61
1	J	165/178 (93%)	159 (96%)	6 (4%)	35	61
1	L	165/178 (93%)	160 (97%)	5 (3%)	41	68
1	N	165/178 (93%)	161 (98%)	4 (2%)	49	74
1	P	165/178 (93%)	160 (97%)	5 (3%)	41	68
1	R	165/178 (93%)	160 (97%)	5 (3%)	41	68
1	T	165/178 (93%)	160 (97%)	5 (3%)	41	68
1	V	167/178 (94%)	160 (96%)	7 (4%)	30	54
1	X	165/178 (93%)	160 (97%)	5 (3%)	41	68
1	Z	165/178 (93%)	160 (97%)	5 (3%)	41	68
2	1	164/184 (89%)	156 (95%)	8 (5%)	25	47
2	A	164/184 (89%)	156 (95%)	8 (5%)	25	47
2	B	164/184 (89%)	154 (94%)	10 (6%)	18	36
2	D	163/184 (89%)	156 (96%)	7 (4%)	29	53
2	F	164/184 (89%)	154 (94%)	10 (6%)	18	36
2	I	164/184 (89%)	153 (93%)	11 (7%)	16	31
2	K	164/184 (89%)	154 (94%)	10 (6%)	18	36
2	M	164/184 (89%)	153 (93%)	11 (7%)	16	31
2	O	164/184 (89%)	155 (94%)	9 (6%)	21	41
2	Q	164/184 (89%)	156 (95%)	8 (5%)	25	47
2	S	164/184 (89%)	156 (95%)	8 (5%)	25	47
2	U	164/184 (89%)	153 (93%)	11 (7%)	16	31

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	W	164/184 (89%)	154 (94%)	10 (6%)	18	36
2	Y	164/184 (89%)	157 (96%)	7 (4%)	29	53
All	All	4607/5068 (91%)	4403 (96%)	204 (4%)	28	52

All (204) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	363	LEU
1	H	374	LEU
1	H	402	PRO
1	H	461	ASP
1	H	471	LEU
1	H	513	LEU
1	C	363	LEU
1	C	374	LEU
1	C	461	ASP
1	C	471	LEU
1	C	496	ILE
1	C	513	LEU
1	E	363	LEU
1	E	374	LEU
1	E	461	ASP
1	E	471	LEU
1	E	513	LEU
1	G	337	THR
1	G	363	LEU
1	G	374	LEU
1	G	461	ASP
1	G	471	LEU
1	G	496	ILE
1	G	513	LEU
1	J	363	LEU
1	J	374	LEU
1	J	444	LEU
1	J	461	ASP
1	J	471	LEU
1	J	513	LEU
1	L	363	LEU
1	L	374	LEU
1	L	461	ASP
1	L	471	LEU

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Mol	Chain	Res	Type
1	L	513	LEU
1	N	363	LEU
1	N	374	LEU
1	N	461	ASP
1	N	513	LEU
1	P	363	LEU
1	P	374	LEU
1	P	461	ASP
1	P	471	LEU
1	P	513	LEU
1	R	363	LEU
1	R	374	LEU
1	R	402	PRO
1	R	461	ASP
1	R	471	LEU
1	T	363	LEU
1	T	374	LEU
1	T	461	ASP
1	T	471	LEU
1	T	513	LEU
1	V	363	LEU
1	V	374	LEU
1	V	461	ASP
1	V	471	LEU
1	V	496	ILE
1	V	513	LEU
1	V	526	THR
1	X	363	LEU
1	X	374	LEU
1	X	461	ASP
1	X	471	LEU
1	X	513	LEU
1	Z	363	LEU
1	Z	374	LEU
1	Z	461	ASP
1	Z	471	LEU
1	Z	513	LEU
1	2	363	LEU
1	2	374	LEU
1	2	461	ASP
1	2	471	LEU
1	2	513	LEU

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Mol	Chain	Res	Type
2	D	52	LYS
2	D	59	ARG
2	D	102	VAL
2	D	133	THR
2	D	135	ARG
2	D	140	ARG
2	D	167	LEU
2	A	52	LYS
2	A	99	LEU
2	A	102	VAL
2	A	133	THR
2	A	135	ARG
2	A	140	ARG
2	A	167	LEU
2	A	234	LEU
2	B	9	MET
2	B	51	GLN
2	B	102	VAL
2	B	105	GLN
2	B	107	LEU
2	B	144	ASP
2	B	176	SER
2	B	217	ARG
2	B	230	LEU
2	B	234	LEU
2	F	52	LYS
2	F	59	ARG
2	F	99	LEU
2	F	102	VAL
2	F	133	THR
2	F	135	ARG
2	F	140	ARG
2	F	167	LEU
2	F	203	LEU
2	F	234	LEU
2	I	52	LYS
2	I	57	TYR
2	I	59	ARG
2	I	69	ASN
2	I	133	THR
2	I	135	ARG
2	I	140	ARG

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Mol	Chain	Res	Type
2	I	167	LEU
2	I	188	LEU
2	I	203	LEU
2	I	212	VAL
2	K	52	LYS
2	K	59	ARG
2	K	69	ASN
2	K	99	LEU
2	K	102	VAL
2	K	133	THR
2	K	135	ARG
2	K	140	ARG
2	K	167	LEU
2	K	188	LEU
2	M	48	ARG
2	M	52	LYS
2	M	59	ARG
2	M	99	LEU
2	M	102	VAL
2	M	133	THR
2	M	135	ARG
2	M	140	ARG
2	M	167	LEU
2	M	233	LEU
2	M	234	LEU
2	O	52	LYS
2	O	59	ARG
2	O	102	VAL
2	O	133	THR
2	O	135	ARG
2	O	140	ARG
2	O	167	LEU
2	O	188	LEU
2	O	234	LEU
2	Q	52	LYS
2	Q	99	LEU
2	Q	102	VAL
2	Q	133	THR
2	Q	135	ARG
2	Q	140	ARG
2	Q	167	LEU
2	Q	234	LEU

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Mol	Chain	Res	Type
2	S	52	LYS
2	S	59	ARG
2	S	102	VAL
2	S	133	THR
2	S	135	ARG
2	S	140	ARG
2	S	167	LEU
2	S	234	LEU
2	U	9	MET
2	U	52	LYS
2	U	69	ASN
2	U	99	LEU
2	U	102	VAL
2	U	133	THR
2	U	135	ARG
2	U	140	ARG
2	U	231	GLN
2	U	233	LEU
2	U	234	LEU
2	W	10	GLU
2	W	52	LYS
2	W	59	ARG
2	W	69	ASN
2	W	102	VAL
2	W	133	THR
2	W	135	ARG
2	W	140	ARG
2	W	167	LEU
2	W	234	LEU
2	Y	52	LYS
2	Y	59	ARG
2	Y	99	LEU
2	Y	102	VAL
2	Y	140	ARG
2	Y	167	LEU
2	Y	188	LEU
2	1	9	MET
2	1	48	ARG
2	1	52	LYS
2	1	99	LEU
2	1	102	VAL
2	1	133	THR

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Mol	Chain	Res	Type
2	1	135	ARG
2	1	140	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (74) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	396	GLN
1	H	456	GLN
1	C	396	GLN
1	C	456	GLN
1	E	396	GLN
1	E	456	GLN
1	G	396	GLN
1	G	456	GLN
1	J	396	GLN
1	J	456	GLN
1	L	396	GLN
1	L	456	GLN
1	N	396	GLN
1	N	456	GLN
1	P	396	GLN
1	P	456	GLN
1	R	396	GLN
1	R	456	GLN
1	T	396	GLN
1	T	456	GLN
1	V	396	GLN
1	V	456	GLN
1	X	396	GLN
1	X	456	GLN
1	Z	396	GLN
1	Z	456	GLN
1	2	396	GLN
1	2	430	ASN
1	2	456	GLN
2	D	69	ASN
2	D	73	ASN
2	D	98	GLN
2	D	129	HIS
2	A	69	ASN
2	A	73	ASN
2	A	98	GLN

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Mol	Chain	Res	Type
2	A	129	HIS
2	B	105	GLN
2	B	174	ASN
2	F	69	ASN
2	F	98	GLN
2	F	129	HIS
2	I	69	ASN
2	I	73	ASN
2	I	105	GLN
2	I	129	HIS
2	K	69	ASN
2	K	129	HIS
2	M	69	ASN
2	M	98	GLN
2	M	114	GLN
2	M	129	HIS
2	O	69	ASN
2	O	98	GLN
2	O	105	GLN
2	O	129	HIS
2	Q	11	GLN
2	Q	69	ASN
2	Q	98	GLN
2	S	69	ASN
2	S	98	GLN
2	S	129	HIS
2	U	69	ASN
2	U	98	GLN
2	U	129	HIS
2	W	69	ASN
2	W	98	GLN
2	W	129	HIS
2	Y	69	ASN
2	Y	98	GLN
2	Y	129	HIS
2	1	69	ASN
2	1	98	GLN
2	1	129	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

58 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	S	250	-	4,4,4	0.35	0	4,4,4	0.34	0
3	DMF	1	250	-	4,4,4	0.37	0	4,4,4	0.47	0
3	DMF	G	137	-	4,4,4	0.35	0	4,4,4	0.44	0
3	DMF	2	99	-	4,4,4	0.34	0	4,4,4	0.44	0
3	DMF	Z	27	-	4,4,4	0.34	0	4,4,4	0.43	0
3	DMF	N	36	-	4,4,4	0.36	0	4,4,4	0.40	0
3	DMF	Z	122	-	4,4,4	0.34	0	4,4,4	0.37	0
3	DMF	P	107	-	4,4,4	0.28	0	4,4,4	0.41	0
3	DMF	V	117	-	4,4,4	0.38	0	4,4,4	0.42	0
3	DMF	L	14	-	4,4,4	0.36	0	4,4,4	0.32	0
3	DMF	E	113	-	4,4,4	0.37	0	4,4,4	0.48	0
3	DMF	1	249	-	4,4,4	0.37	0	4,4,4	0.25	0
3	DMF	J	46	-	4,4,4	0.36	0	4,4,4	0.49	0
3	DMF	Z	50	-	4,4,4	0.34	0	4,4,4	0.39	0
3	DMF	2	145	-	4,4,4	0.31	0	4,4,4	0.42	0
3	DMF	U	249	-	4,4,4	0.33	0	4,4,4	0.33	0
3	DMF	Q	250	-	4,4,4	0.35	0	4,4,4	0.26	0
3	DMF	K	251	-	4,4,4	0.35	0	4,4,4	0.26	0
3	DMF	F	249	-	4,4,4	0.33	0	4,4,4	0.41	0
3	DMF	K	249	-	4,4,4	0.30	0	4,4,4	0.30	0
3	DMF	M	249	-	4,4,4	0.37	0	4,4,4	0.36	0
3	DMF	Y	250	-	4,4,4	0.29	0	4,4,4	0.40	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	DMF	S	249	-	4,4,4	0.31	0	4,4,4	0.30	0
3	DMF	U	250	-	4,4,4	0.31	0	4,4,4	0.31	0
3	DMF	N	21	-	4,4,4	0.31	0	4,4,4	0.42	0
3	DMF	V	135	-	4,4,4	0.40	0	4,4,4	0.44	0
3	DMF	Q	249	-	4,4,4	0.32	0	4,4,4	0.35	0
3	DMF	H	41	-	4,4,4	0.32	0	4,4,4	0.45	0
3	DMF	Y	251	-	4,4,4	0.39	0	4,4,4	0.45	0
3	DMF	V	16	-	4,4,4	0.35	0	4,4,4	0.39	0
3	DMF	V	136	-	4,4,4	0.40	0	4,4,4	0.46	0
3	DMF	Y	249	-	4,4,4	0.47	0	4,4,4	0.55	0
3	DMF	C	15	-	4,4,4	0.32	0	4,4,4	0.39	0
3	DMF	L	9	-	4,4,4	0.36	0	4,4,4	0.45	0
3	DMF	G	140	-	4,4,4	0.35	0	4,4,4	0.48	0
3	DMF	A	8	-	4,4,4	0.25	0	4,4,4	0.27	0
3	DMF	A	249	-	4,4,4	0.39	0	4,4,4	0.49	0
3	DMF	Q	251	-	4,4,4	0.31	0	4,4,4	0.43	0
3	DMF	L	60	-	4,4,4	0.33	0	4,4,4	0.44	0
3	DMF	O	7	-	4,4,4	0.37	0	4,4,4	0.38	0
3	DMF	Z	69	-	4,4,4	0.35	0	4,4,4	0.34	0
3	DMF	I	249	-	4,4,4	0.31	0	4,4,4	0.42	0
3	DMF	X	141	-	4,4,4	0.30	0	4,4,4	0.34	0
3	DMF	G	20	-	4,4,4	0.36	0	4,4,4	0.24	0
3	DMF	V	121	-	4,4,4	0.36	0	4,4,4	0.55	0
3	DMF	B	249	-	4,4,4	0.31	0	4,4,4	0.44	0
3	DMF	D	249	-	4,4,4	0.32	0	4,4,4	0.47	0
3	DMF	P	133	-	4,4,4	0.34	0	4,4,4	0.46	0
3	DMF	Z	105	-	4,4,4	0.38	0	4,4,4	0.37	0
3	DMF	T	134	-	4,4,4	0.34	0	4,4,4	0.46	0
3	DMF	L	138	-	4,4,4	0.36	0	4,4,4	0.29	0
3	DMF	E	28	-	4,4,4	0.36	0	4,4,4	0.38	0
3	DMF	W	249	-	4,4,4	0.29	0	4,4,4	0.20	0
3	DMF	E	104	-	4,4,4	0.28	0	4,4,4	0.43	0
3	DMF	K	250	-	4,4,4	0.38	0	4,4,4	0.43	0
3	DMF	T	62	-	4,4,4	0.33	0	4,4,4	0.36	0
3	DMF	P	23	-	4,4,4	0.32	0	4,4,4	0.40	0
3	DMF	H	142	-	4,4,4	0.37	0	4,4,4	0.49	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	S	250	-	-	2/2/2/2	-
3	DMF	1	250	-	-	0/2/2/2	-
3	DMF	G	137	-	-	2/2/2/2	-
3	DMF	2	99	-	-	2/2/2/2	-
3	DMF	Z	27	-	-	2/2/2/2	-
3	DMF	N	36	-	-	0/2/2/2	-
3	DMF	Z	122	-	-	2/2/2/2	-
3	DMF	P	107	-	-	2/2/2/2	-
3	DMF	V	117	-	-	0/2/2/2	-
3	DMF	L	14	-	-	2/2/2/2	-
3	DMF	E	113	-	-	1/2/2/2	-
3	DMF	1	249	-	-	2/2/2/2	-
3	DMF	J	46	-	-	0/2/2/2	-
3	DMF	Z	50	-	-	2/2/2/2	-
3	DMF	2	145	-	-	2/2/2/2	-
3	DMF	U	249	-	-	2/2/2/2	-
3	DMF	Q	250	-	-	0/2/2/2	-
3	DMF	K	251	-	-	1/2/2/2	-
3	DMF	F	249	-	-	2/2/2/2	-
3	DMF	K	249	-	-	2/2/2/2	-
3	DMF	M	249	-	-	0/2/2/2	-
3	DMF	Y	250	-	-	0/2/2/2	-
3	DMF	S	249	-	-	2/2/2/2	-
3	DMF	U	250	-	-	2/2/2/2	-
3	DMF	N	21	-	-	2/2/2/2	-
3	DMF	V	135	-	-	2/2/2/2	-
3	DMF	Q	249	-	-	0/2/2/2	-
3	DMF	H	41	-	-	2/2/2/2	-
3	DMF	Y	251	-	-	2/2/2/2	-
3	DMF	V	16	-	-	2/2/2/2	-
3	DMF	V	136	-	-	0/2/2/2	-
3	DMF	Y	249	-	-	2/2/2/2	-
3	DMF	C	15	-	-	2/2/2/2	-
3	DMF	L	9	-	-	0/2/2/2	-
3	DMF	G	140	-	-	2/2/2/2	-
3	DMF	A	8	-	-	0/2/2/2	-
3	DMF	A	249	-	-	0/2/2/2	-
3	DMF	Q	251	-	-	2/2/2/2	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	DMF	L	60	-	-	2/2/2/2	-
3	DMF	O	7	-	-	0/2/2/2	-
3	DMF	Z	69	-	-	2/2/2/2	-
3	DMF	I	249	-	-	2/2/2/2	-
3	DMF	X	141	-	-	0/2/2/2	-
3	DMF	G	20	-	-	2/2/2/2	-
3	DMF	V	121	-	-	0/2/2/2	-
3	DMF	B	249	-	-	1/2/2/2	-
3	DMF	D	249	-	-	0/2/2/2	-
3	DMF	P	133	-	-	2/2/2/2	-
3	DMF	Z	105	-	-	0/2/2/2	-
3	DMF	T	134	-	-	0/2/2/2	-
3	DMF	L	138	-	-	2/2/2/2	-
3	DMF	E	28	-	-	2/2/2/2	-
3	DMF	W	249	-	-	2/2/2/2	-
3	DMF	E	104	-	-	2/2/2/2	-
3	DMF	K	250	-	-	2/2/2/2	-
3	DMF	T	62	-	-	0/2/2/2	-
3	DMF	P	23	-	-	2/2/2/2	-
3	DMF	H	142	-	-	2/2/2/2	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (75) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	2	99	DMF	O-C-N-C2
3	Q	251	DMF	O-C-N-C2
3	2	99	DMF	O-C-N-C1
3	Q	251	DMF	O-C-N-C1
3	U	249	DMF	O-C-N-C2
3	G	137	DMF	O-C-N-C1
3	L	14	DMF	O-C-N-C1
3	U	249	DMF	O-C-N-C1
3	Y	251	DMF	O-C-N-C1
3	V	16	DMF	O-C-N-C1
3	I	249	DMF	O-C-N-C1

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Mol	Chain	Res	Type	Atoms
3	G	137	DMF	O-C-N-C2
3	V	16	DMF	O-C-N-C2
3	Z	69	DMF	O-C-N-C1
3	W	249	DMF	O-C-N-C2
3	Z	69	DMF	O-C-N-C2
3	W	249	DMF	O-C-N-C1
3	Y	251	DMF	O-C-N-C2
3	Z	50	DMF	O-C-N-C1
3	C	15	DMF	O-C-N-C1
3	L	14	DMF	O-C-N-C2
3	F	249	DMF	O-C-N-C2
3	P	133	DMF	O-C-N-C1
3	1	249	DMF	O-C-N-C1
3	I	249	DMF	O-C-N-C2
3	K	250	DMF	O-C-N-C1
3	Z	50	DMF	O-C-N-C2
3	F	249	DMF	O-C-N-C1
3	C	15	DMF	O-C-N-C2
3	P	133	DMF	O-C-N-C2
3	1	249	DMF	O-C-N-C2
3	G	20	DMF	O-C-N-C1
3	K	249	DMF	O-C-N-C1
3	Z	27	DMF	O-C-N-C1
3	P	23	DMF	O-C-N-C1
3	N	21	DMF	O-C-N-C1
3	2	145	DMF	O-C-N-C1
3	K	250	DMF	O-C-N-C2
3	K	249	DMF	O-C-N-C2
3	G	20	DMF	O-C-N-C2
3	Z	27	DMF	O-C-N-C2
3	P	23	DMF	O-C-N-C2
3	V	135	DMF	O-C-N-C1
3	S	250	DMF	O-C-N-C1
3	U	250	DMF	O-C-N-C1
3	H	41	DMF	O-C-N-C1
3	N	21	DMF	O-C-N-C2
3	2	145	DMF	O-C-N-C2
3	L	60	DMF	O-C-N-C1
3	Z	122	DMF	O-C-N-C1
3	L	138	DMF	O-C-N-C1
3	S	249	DMF	O-C-N-C1
3	P	107	DMF	O-C-N-C1

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Mol	Chain	Res	Type	Atoms
3	E	104	DMF	O-C-N-C1
3	S	250	DMF	O-C-N-C2
3	V	135	DMF	O-C-N-C2
3	U	250	DMF	O-C-N-C2
3	H	41	DMF	O-C-N-C2
3	Y	249	DMF	O-C-N-C1
3	Z	122	DMF	O-C-N-C2
3	L	60	DMF	O-C-N-C2
3	S	249	DMF	O-C-N-C2
3	L	138	DMF	O-C-N-C2
3	E	104	DMF	O-C-N-C2
3	P	107	DMF	O-C-N-C2
3	Y	249	DMF	O-C-N-C2
3	E	28	DMF	O-C-N-C1
3	E	28	DMF	O-C-N-C2
3	G	140	DMF	O-C-N-C1
3	H	142	DMF	O-C-N-C1
3	G	140	DMF	O-C-N-C2
3	K	251	DMF	O-C-N-C1
3	B	249	DMF	O-C-N-C1
3	E	113	DMF	O-C-N-C1
3	H	142	DMF	O-C-N-C2

There are no ring outliers.

32 monomers are involved in 55 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	137	DMF	1	0
3	2	99	DMF	1	0
3	P	107	DMF	2	0
3	V	117	DMF	1	0
3	E	113	DMF	1	0
3	1	249	DMF	2	0
3	2	145	DMF	1	0
3	U	249	DMF	1	0
3	K	251	DMF	4	0
3	K	249	DMF	1	0
3	S	249	DMF	1	0
3	N	21	DMF	1	0
3	V	135	DMF	1	0
3	V	16	DMF	1	0
3	V	136	DMF	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	Y	249	DMF	1	0
3	L	9	DMF	1	0
3	G	140	DMF	2	0
3	A	249	DMF	1	0
3	Q	251	DMF	5	0
3	Z	69	DMF	5	0
3	I	249	DMF	1	0
3	G	20	DMF	1	0
3	V	121	DMF	3	0
3	P	133	DMF	1	0
3	Z	105	DMF	2	0
3	T	134	DMF	2	0
3	L	138	DMF	3	0
3	W	249	DMF	1	0
3	E	104	DMF	3	0
3	T	62	DMF	3	0
3	H	142	DMF	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	2	222/240 (92%)	-0.35	1 (0%) 91 91	17, 32, 63, 84	0
1	C	222/240 (92%)	0.52	12 (5%) 25 27	26, 43, 72, 89	0
1	E	223/240 (92%)	-0.19	6 (2%) 54 58	19, 32, 67, 134	0
1	G	222/240 (92%)	-0.28	0 100 100	18, 28, 62, 83	0
1	H	223/240 (92%)	0.05	4 (1%) 68 71	22, 36, 65, 86	0
1	J	222/240 (92%)	0.10	10 (4%) 33 36	24, 38, 71, 89	0
1	L	222/240 (92%)	-0.37	4 (1%) 68 71	18, 30, 64, 83	0
1	N	223/240 (92%)	-0.39	1 (0%) 92 93	15, 30, 64, 118	0
1	P	222/240 (92%)	-0.20	4 (1%) 68 71	19, 33, 67, 85	0
1	R	222/240 (92%)	-0.14	3 (1%) 75 77	22, 34, 66, 84	0
1	T	223/240 (92%)	-0.26	1 (0%) 92 93	21, 33, 67, 98	0
1	V	226/240 (94%)	-0.39	2 (0%) 84 86	16, 29, 65, 81	0
1	X	224/240 (93%)	-0.29	4 (1%) 68 71	19, 30, 66, 124	0
1	Z	224/240 (93%)	-0.24	0 100 100	21, 34, 68, 107	0
2	1	214/240 (89%)	0.11	6 (2%) 53 56	25, 48, 89, 127	0
2	A	214/240 (89%)	1.29	52 (24%) 0 0	37, 64, 111, 131	0
2	B	214/240 (89%)	1.77	83 (38%) 0 0	40, 87, 134, 168	0
2	D	213/240 (88%)	0.28	18 (8%) 10 10	24, 49, 98, 124	0
2	F	214/240 (89%)	0.33	20 (9%) 8 8	24, 48, 96, 127	0
2	I	214/240 (89%)	0.78	26 (12%) 4 4	34, 53, 98, 125	0
2	K	214/240 (89%)	0.37	15 (7%) 16 16	25, 49, 92, 126	0
2	M	214/240 (89%)	-0.02	5 (2%) 60 63	22, 45, 90, 124	0
2	O	214/240 (89%)	0.42	18 (8%) 11 11	26, 54, 95, 129	0
2	Q	214/240 (89%)	0.03	9 (4%) 36 39	20, 42, 90, 126	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
2	S	214/240 (89%)	0.65	29 (13%) 3 2	28, 53, 98, 126	0
2	U	214/240 (89%)	0.33	14 (6%) 18 19	22, 51, 99, 126	0
2	W	214/240 (89%)	0.24	11 (5%) 28 29	22, 46, 94, 125	0
2	Y	214/240 (89%)	0.18	10 (4%) 31 33	23, 46, 90, 127	0
All	All	6115/6720 (90%)	0.15	368 (6%) 21 22	15, 40, 90, 168	0

All (368) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	U	234	LEU	8.0
2	A	9	MET	7.5
2	A	203	LEU	6.8
2	Y	9	MET	6.7
2	1	9	MET	6.5
2	A	233	LEU	6.4
2	B	205	VAL	6.4
2	B	42	VAL	6.2
2	B	40	LEU	6.2
2	B	179	ASP	6.0
2	B	180	ALA	6.0
2	B	41	PHE	6.0
2	B	36	ALA	5.9
2	F	233	LEU	5.7
2	A	205	VAL	5.7
2	B	38	GLY	5.6
2	U	206	ALA	5.5
2	B	9	MET	5.5
2	I	203	LEU	5.3
2	D	204	GLY	5.3
2	S	205	VAL	5.3
2	S	203	LEU	5.2
2	A	178	THR	5.1
2	O	231	GLN	5.0
2	A	231	GLN	5.0
2	Q	169	GLU	4.8
2	B	211	ALA	4.8
2	I	205	VAL	4.8
2	B	33	LEU	4.7
2	O	205	VAL	4.7
2	A	13	MET	4.6
2	D	205	VAL	4.6

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Mol	Chain	Res	Type	RSRZ
2	Q	9	MET	4.5
2	I	9	MET	4.5
2	B	31	VAL	4.5
2	Y	203	LEU	4.5
2	S	9	MET	4.5
2	D	206	ALA	4.5
2	Y	10	GLU	4.5
2	B	230	LEU	4.4
2	F	9	MET	4.4
2	U	203	LEU	4.3
2	B	35	TYR	4.3
2	Y	169	GLU	4.2
2	A	179	ASP	4.1
2	A	234	LEU	4.1
2	I	230	LEU	4.1
2	B	37	GLY	4.1
2	A	171	TYR	4.1
2	S	234	LEU	4.1
2	B	44	GLU	4.1
2	B	169	GLU	4.1
2	1	12	ALA	4.0
2	B	222	PHE	4.0
2	A	227	GLY	4.0
2	B	61	GLY	4.0
2	B	39	VAL	4.0
2	D	182	ARG	4.0
2	A	182	ARG	4.0
2	B	213	LEU	4.0
2	B	34	ALA	3.9
2	S	162	PRO	3.9
2	F	10	GLU	3.9
2	A	20	ALA	3.9
1	J	414	PRO	3.9
2	M	9	MET	3.8
2	W	232	ALA	3.8
2	O	203	LEU	3.8
2	S	228	SER	3.8
2	F	227	GLY	3.8
2	B	60	VAL	3.8
2	B	182	ARG	3.8
2	O	204	GLY	3.7
2	U	205	VAL	3.7

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Mol	Chain	Res	Type	RSRZ
2	B	62	PHE	3.7
2	B	234	LEU	3.7
1	J	415	GLN	3.6
2	W	182	ARG	3.6
2	B	212	VAL	3.6
1	X	523	GLY	3.6
2	A	168	LYS	3.6
2	S	169	GLU	3.5
2	B	133	THR	3.5
2	B	127	VAL	3.5
2	Q	131	GLY	3.5
2	I	135	ARG	3.5
1	C	501	GLY	3.5
2	A	165	ASN	3.5
2	B	153	PHE	3.5
2	B	48	ARG	3.5
1	C	409	ILE	3.4
2	B	64	ALA	3.4
2	A	229	ALA	3.4
2	B	232	ALA	3.4
2	O	9	MET	3.4
2	S	171	TYR	3.4
2	W	48	ARG	3.4
2	A	169	GLU	3.4
2	A	161	GLU	3.4
2	K	203	LEU	3.3
2	I	182	ARG	3.3
2	B	208	LEU	3.3
2	K	26	ARG	3.3
2	B	181	LEU	3.3
2	I	177	LEU	3.3
1	C	340	TYR	3.3
2	B	171	TYR	3.3
2	F	11	GLN	3.3
2	Y	205	VAL	3.3
2	B	32	ALA	3.2
1	E	523	GLY	3.2
2	A	218	PRO	3.2
2	B	53	ILE	3.2
2	O	48	ARG	3.2
2	B	218	PRO	3.2
2	B	225	ILE	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	415	GLN	3.1
2	I	172	ALA	3.1
2	F	178	THR	3.1
2	W	203	LEU	3.1
2	A	189	ARG	3.1
2	B	168	LYS	3.1
1	J	413	ASP	3.1
1	C	519	GLU	3.1
2	Q	130	TYR	3.1
2	U	169	GLU	3.1
2	K	205	VAL	3.1
2	K	11	GLN	3.0
2	B	210	VAL	3.0
2	W	205	VAL	3.0
2	B	130	TYR	3.0
2	F	171	TYR	3.0
2	I	171	TYR	3.0
2	I	38	GLY	3.0
2	B	215	ALA	3.0
2	B	226	THR	3.0
2	F	203	LEU	3.0
2	A	11	GLN	3.0
1	J	412	SER	3.0
2	D	169	GLU	3.0
2	O	227	GLY	3.0
2	K	25	ALA	3.0
1	H	372	VAL	3.0
2	Q	10	GLU	3.0
2	D	189	ARG	3.0
2	A	135	ARG	3.0
2	B	123	CYS	2.9
2	W	9	MET	2.9
2	B	54	SER	2.9
2	B	227	GLY	2.9
1	N	523	GLY	2.9
1	X	524	ALA	2.9
2	O	10	GLU	2.9
2	O	234	LEU	2.9
2	B	30	VAL	2.9
1	R	412	SER	2.8
2	B	223	ARG	2.8
1	2	415	GLN	2.8

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Mol	Chain	Res	Type	RSRZ
2	A	170	SER	2.8
2	B	52	LYS	2.8
2	F	168	LYS	2.8
2	B	184	ALA	2.8
2	I	128	ALA	2.8
2	A	207	SER	2.8
1	C	407	TYR	2.8
2	A	12	ALA	2.8
2	O	11	GLN	2.8
2	U	207	SER	2.8
2	F	205	VAL	2.8
2	A	130	TYR	2.8
2	A	159	THR	2.8
2	B	51	GLN	2.8
2	B	63	ALA	2.8
2	I	229	ALA	2.8
2	A	124	VAL	2.8
2	O	233	LEU	2.8
2	I	189	ARG	2.8
2	B	172	ALA	2.7
2	W	172	ALA	2.7
1	C	412	SER	2.7
2	A	188	LEU	2.7
2	D	161	GLU	2.7
2	B	160	THR	2.7
1	V	526	THR	2.7
2	F	206	ALA	2.7
2	I	228	SER	2.7
2	Q	203	LEU	2.7
2	Q	231	GLN	2.7
2	B	209	GLU	2.7
2	K	216	ASN	2.7
2	W	169	GLU	2.7
2	U	216	ASN	2.7
2	A	180	ALA	2.7
2	B	173	GLU	2.7
2	D	234	LEU	2.7
1	V	523	GLY	2.7
2	S	227	GLY	2.7
2	1	10	GLU	2.6
2	A	123	CYS	2.6
2	O	206	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
2	A	204	GLY	2.6
2	O	169	GLU	2.6
2	A	172	ALA	2.6
2	F	226	THR	2.6
2	S	36	ALA	2.6
2	S	37	GLY	2.6
2	Y	227	GLY	2.6
1	R	413	ASP	2.6
2	B	154	VAL	2.6
1	H	412	SER	2.6
2	O	168	LYS	2.6
2	B	186	ALA	2.6
2	O	229	ALA	2.6
1	J	522	SER	2.6
1	L	412	SER	2.6
2	B	175	ALA	2.5
1	J	506	PRO	2.5
2	F	231	GLN	2.5
2	A	175	ALA	2.5
2	A	216	ASN	2.5
2	B	165	ASN	2.5
2	I	133	THR	2.5
2	D	233	LEU	2.5
2	A	176	SER	2.5
2	A	160	THR	2.5
2	B	221	ALA	2.5
2	F	131	GLY	2.5
2	D	168	LYS	2.5
2	S	163	ILE	2.5
2	K	21	ARG	2.5
2	A	43	ALA	2.5
2	I	10	GLU	2.5
1	P	411	ALA	2.5
2	A	133	THR	2.5
2	I	37	GLY	2.5
2	O	158	GLY	2.5
2	S	135	ARG	2.4
1	C	411	ALA	2.4
2	U	130	TYR	2.4
2	A	230	LEU	2.4
2	B	203	LEU	2.4
2	S	167	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
2	Q	135	ARG	2.4
2	W	206	ALA	2.4
1	J	519	GLU	2.4
2	M	172	ALA	2.4
2	S	159	THR	2.4
2	1	232	ALA	2.4
2	B	189	ARG	2.4
2	B	216	ASN	2.4
2	B	12	ALA	2.4
1	J	503	VAL	2.4
2	1	130	TYR	2.4
2	A	25	ALA	2.4
1	X	415	GLN	2.4
2	B	159	THR	2.4
2	S	158	GLY	2.3
1	C	414	PRO	2.3
2	B	183	ILE	2.3
2	F	48	ARG	2.3
2	F	229	ALA	2.3
2	F	230	LEU	2.3
2	S	204	GLY	2.3
2	Y	204	GLY	2.3
2	B	152	HIS	2.3
2	S	189	ARG	2.3
2	S	21	ARG	2.3
2	I	153	PHE	2.3
1	J	416	SER	2.3
2	S	182	ARG	2.3
2	F	130	TYR	2.3
1	E	414	PRO	2.3
1	C	510	ILE	2.3
2	K	48	ARG	2.3
2	B	125	ALA	2.3
2	D	133	THR	2.3
2	A	208	LEU	2.3
2	S	10	GLU	2.3
2	A	174	ASN	2.3
1	R	417	ALA	2.3
2	D	232	ALA	2.3
2	S	179	ASP	2.3
2	K	133	THR	2.3
2	S	161	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
2	I	204	GLY	2.2
1	P	519	GLU	2.2
2	A	44	GLU	2.2
2	B	138	LEU	2.2
1	L	414	PRO	2.2
1	P	414	PRO	2.2
2	O	46	PRO	2.2
2	B	26	ARG	2.2
2	Q	171	TYR	2.2
2	K	18	GLU	2.2
2	A	14	ARG	2.2
2	D	230	LEU	2.2
2	D	159	THR	2.2
2	D	178	THR	2.2
2	A	10	GLU	2.2
2	U	233	LEU	2.2
2	D	48	ARG	2.2
2	W	189	ARG	2.2
1	X	411	ALA	2.2
2	U	232	ALA	2.2
2	Y	189	ARG	2.2
2	K	9	MET	2.2
2	B	206	ALA	2.2
1	J	500	ASP	2.2
2	A	163	ILE	2.2
2	I	133	THR	2.2
2	B	224	ARG	2.2
2	M	169	GLU	2.2
2	B	164	ALA	2.1
2	F	172	ALA	2.1
2	U	157	GLY	2.1
2	B	50	LEU	2.1
2	I	233	LEU	2.1
2	S	208	LEU	2.1
2	S	168	LYS	2.1
1	H	396	GLN	2.1
1	T	415	GLN	2.1
2	W	231	GLN	2.1
2	K	206	ALA	2.1
2	A	62	PHE	2.1
2	B	11	GLN	2.1
2	B	207	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	500	ASP	2.1
2	I	214	ASP	2.1
1	L	519	GLU	2.1
1	C	397	GLY	2.1
2	U	131	GLY	2.1
1	P	415	GLN	2.1
2	U	231	GLN	2.1
2	Y	231	GLN	2.1
1	L	413	ASP	2.1
2	I	169	GLU	2.1
2	Y	174	ASN	2.1
1	E	411	ALA	2.1
2	B	229	ALA	2.1
2	F	232	ALA	2.1
2	I	190	ALA	2.1
2	K	130	TYR	2.1
2	U	163	ILE	2.1
2	A	177	LEU	2.1
2	I	14	ARG	2.1
2	I	179	ASP	2.1
2	S	230	LEU	2.1
2	M	234	LEU	2.1
2	A	158	GLY	2.1
2	A	173	GLU	2.1
2	I	130	TYR	2.1
2	D	228	SER	2.1
2	B	167	LEU	2.1
2	K	228	SER	2.1
2	S	12	ALA	2.0
1	E	412	SER	2.0
2	K	10	GLU	2.0
2	D	14	ARG	2.0
2	S	13	MET	2.0
1	H	411	ALA	2.0
2	M	10	GLU	2.0
2	B	49	SER	2.0
2	S	130	TYR	2.0
1	E	397	GLY	2.0
2	O	189	ARG	2.0
1	E	415	GLN	2.0
2	A	151	PRO	2.0
2	B	156	MET	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. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	DMF	V	135	5/5	0.78	0.34	35,51,75,87	0
3	DMF	Z	69	5/5	0.82	0.34	53,80,102,104	0
3	DMF	Z	50	5/5	0.86	0.40	86,90,126,146	0
3	DMF	V	117	5/5	0.86	0.24	46,50,66,72	0
3	DMF	Y	251	5/5	0.86	0.26	42,45,61,63	0
3	DMF	L	9	5/5	0.86	0.33	53,54,82,89	0
3	DMF	L	14	5/5	0.86	0.41	30,38,70,90	0
3	DMF	1	250	5/5	0.88	0.22	43,63,73,87	0
3	DMF	G	20	5/5	0.88	0.30	27,40,70,93	0
3	DMF	K	251	5/5	0.88	0.22	39,50,64,80	0
3	DMF	U	250	5/5	0.89	0.20	50,54,62,63	0
3	DMF	X	141	5/5	0.89	0.37	40,55,82,85	0
3	DMF	E	28	5/5	0.89	0.32	36,68,72,88	0
3	DMF	T	62	5/5	0.89	0.33	45,61,83,95	0
3	DMF	Q	251	5/5	0.90	0.24	26,56,59,84	0
3	DMF	H	142	5/5	0.90	0.27	40,62,68,72	0
3	DMF	Z	27	5/5	0.91	0.25	56,66,86,97	0
3	DMF	V	16	5/5	0.91	0.28	36,61,65,73	0
3	DMF	K	250	5/5	0.91	0.24	42,58,73,78	0
3	DMF	V	136	5/5	0.91	0.24	36,44,59,63	0
3	DMF	Y	249	5/5	0.91	0.21	19,24,64,70	0
3	DMF	P	107	5/5	0.92	0.31	39,58,69,70	0
3	DMF	J	46	5/5	0.92	0.21	29,54,61,63	0
3	DMF	O	7	5/5	0.92	0.21	38,48,59,62	0
3	DMF	C	15	5/5	0.92	0.27	54,69,74,107	0
3	DMF	S	250	5/5	0.92	0.18	26,42,81,85	0
3	DMF	2	145	5/5	0.93	0.22	29,42,52,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	DMF	N	36	5/5	0.93	0.22	35,43,74,83	0
3	DMF	B	249	5/5	0.93	0.28	30,46,52,59	0
3	DMF	P	133	5/5	0.93	0.23	62,69,81,113	0
3	DMF	H	41	5/5	0.93	0.21	53,56,63,80	0
3	DMF	A	8	5/5	0.93	0.20	16,61,76,85	0
3	DMF	S	249	5/5	0.93	0.29	37,57,66,75	0
3	DMF	L	60	5/5	0.93	0.20	35,39,50,58	0
3	DMF	Z	105	5/5	0.93	0.34	22,57,81,82	0
3	DMF	2	99	5/5	0.94	0.17	33,35,64,80	0
3	DMF	L	138	5/5	0.94	0.37	40,47,72,82	0
3	DMF	Z	122	5/5	0.94	0.25	26,28,76,84	0
3	DMF	A	249	5/5	0.94	0.24	23,35,53,58	0
3	DMF	1	249	5/5	0.94	0.26	19,49,53,60	0
3	DMF	E	113	5/5	0.94	0.31	48,56,75,77	0
3	DMF	U	249	5/5	0.95	0.20	11,23,39,54	0
3	DMF	Q	250	5/5	0.95	0.14	23,37,45,58	0
3	DMF	E	104	5/5	0.95	0.26	33,42,51,57	0
3	DMF	N	21	5/5	0.95	0.15	17,53,56,76	0
3	DMF	T	134	5/5	0.96	0.17	33,56,59,79	0
3	DMF	W	249	5/5	0.96	0.16	25,31,39,60	0
3	DMF	V	121	5/5	0.96	0.15	26,27,49,50	0
3	DMF	G	140	5/5	0.96	0.19	24,33,57,59	0
3	DMF	P	23	5/5	0.96	0.20	49,62,83,93	0
3	DMF	D	249	5/5	0.96	0.15	21,22,39,53	0
3	DMF	Y	250	5/5	0.97	0.15	14,36,48,55	0
3	DMF	Q	249	5/5	0.97	0.20	31,39,42,58	0
3	DMF	G	137	5/5	0.97	0.21	27,35,51,57	0
3	DMF	F	249	5/5	0.97	0.13	26,28,37,42	0
3	DMF	M	249	5/5	0.97	0.18	12,15,43,51	0
3	DMF	I	249	5/5	0.98	0.21	41,43,50,58	0
3	DMF	K	249	5/5	0.98	0.12	23,32,46,48	0

6.5 Other polymers ⓘ

There are no such residues in this entry.