



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 1, 2023 – 06:18 AM EDT

PDB ID : 3MFE  
Title : Crystal Structure of Mycobacterium Tuberculosis Proteasome open-gate mutant with H0 movement  
Authors : Li, D.; Li, H.  
Deposited on : 2010-04-02  
Resolution : 2.60 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
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) : 2.36

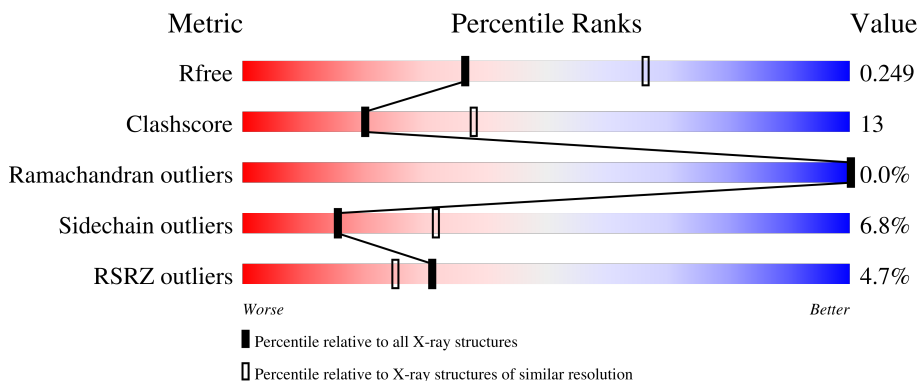
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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 of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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 style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 2px;"></div> <div style="width: 80%; height: 10px; background-color: green; margin-right: 2px;"></div> <div style="width: 11%; height: 10px; background-color: yellow; margin-right: 2px;"></div> <div style="width: 8%; height: 10px; background-color: orange; margin-right: 2px;"></div> <div style="width: 8%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">80%      11%      •      8%</p>
1	C	240	<div style="display: flex; align-items: center;"> <div style="width: 3%; height: 10px; background-color: red; margin-right: 2px;"></div> <div style="width: 74%; height: 10px; background-color: green; margin-right: 2px;"></div> <div style="width: 15%; height: 10px; background-color: yellow; margin-right: 2px;"></div> <div style="width: 8%; height: 10px; background-color: orange; margin-right: 2px;"></div> <div style="width: 8%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">74%      15%      •      8%</p>
1	E	240	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 2px;"></div> <div style="width: 78%; height: 10px; background-color: green; margin-right: 2px;"></div> <div style="width: 13%; height: 10px; background-color: yellow; margin-right: 2px;"></div> <div style="width: 8%; height: 10px; background-color: orange; margin-right: 2px;"></div> <div style="width: 8%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">78%      13%      •      8%</p>
1	H	240	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 2px;"></div> <div style="width: 80%; height: 10px; background-color: green; margin-right: 2px;"></div> <div style="width: 10%; height: 10px; background-color: yellow; margin-right: 2px;"></div> <div style="width: 8%; height: 10px; background-color: orange; margin-right: 2px;"></div> <div style="width: 8%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">80%      10%      •      8%</p>
1	J	240	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 2px;"></div> <div style="width: 81%; height: 10px; background-color: green; margin-right: 2px;"></div> <div style="width: 10%; height: 10px; background-color: yellow; margin-right: 2px;"></div> <div style="width: 8%; height: 10px; background-color: orange; margin-right: 2px;"></div> <div style="width: 8%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">81%      10%      •      8%</p>

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Mol	Chain	Length	Quality of chain
1	L	240	3% 78% 14% • 8%
1	N	240	5% 74% 18% • 8%
1	P	240	2% 79% 12% • 8%
1	R	240	2% 77% 14% • 8%
1	T	240	4% 78% 13% • 8%
1	X	240	4% 79% 12% • 8%
1	Z	240	4% 79% 12% • 8%
2	G	240	1% 78% 14% • 8%
2	V	240	2% 72% 20% • 7%
3	I	240	12% 77% 12% 11%
3	A	240	67% 20% • 11%
3	B	240	67% 22% • 10%
3	D	240	7% 67% 20% • 11%
3	F	240	5% 62% 22% 5% 12%
3	I	240	69% 20% • 10%
3	K	240	66% 22% • 10%
3	M	240	15% 58% 21% • 19%
3	O	240	1% 66% 22% • 11%
3	Q	240	12% 62% 25% • 11%
3	S	240	2% 70% 18% • 10%
3	U	240	15% 62% 26% 12%
3	W	240	8% 58% 27% • 13%
3	Y	240	3% 60% 26% • 11%

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
1	OZT	2	301	-	-	X	-
1	OZT	C	301	-	-	X	-
1	OZT	E	301	-	-	X	-
1	OZT	H	301	-	-	X	-
1	OZT	J	301	-	-	X	-
1	OZT	L	301	-	-	X	-
1	OZT	P	301	-	-	X	-
1	OZT	R	301	-	-	X	-
1	OZT	T	301	-	-	X	-
1	OZT	X	301	-	-	X	-
1	OZT	Z	301	-	-	X	-

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 46890 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Proteasome subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	H	222	1640	1028	282	325	5	0	0	0
1	C	222	1640	1028	282	325	5	0	0	0
1	E	222	1640	1028	282	325	5	0	0	0
1	J	222	1640	1028	282	325	5	0	0	0
1	L	222	1640	1028	282	325	5	0	0	0
1	N	222	1640	1028	282	325	5	0	0	0
1	P	222	1640	1028	282	325	5	0	0	0
1	R	222	1640	1028	282	325	5	0	0	0
1	T	222	1640	1028	282	325	5	0	0	0
1	X	222	1640	1028	282	325	5	0	0	0
1	Z	222	1640	1028	282	325	5	0	0	0
1	2	222	1640	1028	282	325	5	0	0	0

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	301	OZT	-	amidation	UNP O33245
H	535	HIS	-	expression tag	UNP O33245
H	536	HIS	-	expression tag	UNP O33245
H	537	HIS	-	expression tag	UNP O33245
H	538	HIS	-	expression tag	UNP O33245

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Chain	Residue	Modelled	Actual	Comment	Reference
H	539	HIS	-	expression tag	UNP O33245
H	540	HIS	-	expression tag	UNP O33245
C	301	OZT	-	amidation	UNP O33245
C	535	HIS	-	expression tag	UNP O33245
C	536	HIS	-	expression tag	UNP O33245
C	537	HIS	-	expression tag	UNP O33245
C	538	HIS	-	expression tag	UNP O33245
C	539	HIS	-	expression tag	UNP O33245
C	540	HIS	-	expression tag	UNP O33245
E	301	OZT	-	amidation	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
J	301	OZT	-	amidation	UNP O33245
J	535	HIS	-	expression tag	UNP O33245
J	536	HIS	-	expression tag	UNP O33245
J	537	HIS	-	expression tag	UNP O33245
J	538	HIS	-	expression tag	UNP O33245
J	539	HIS	-	expression tag	UNP O33245
J	540	HIS	-	expression tag	UNP O33245
L	301	OZT	-	amidation	UNP O33245
L	535	HIS	-	expression tag	UNP O33245
L	536	HIS	-	expression tag	UNP O33245
L	537	HIS	-	expression tag	UNP O33245
L	538	HIS	-	expression tag	UNP O33245
L	539	HIS	-	expression tag	UNP O33245
L	540	HIS	-	expression tag	UNP O33245
N	301	OZT	-	amidation	UNP O33245
N	535	HIS	-	expression tag	UNP O33245
N	536	HIS	-	expression tag	UNP O33245
N	537	HIS	-	expression tag	UNP O33245
N	538	HIS	-	expression tag	UNP O33245
N	539	HIS	-	expression tag	UNP O33245
N	540	HIS	-	expression tag	UNP O33245
P	301	OZT	-	amidation	UNP O33245
P	535	HIS	-	expression tag	UNP O33245
P	536	HIS	-	expression tag	UNP O33245
P	537	HIS	-	expression tag	UNP O33245
P	538	HIS	-	expression tag	UNP O33245

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Chain	Residue	Modelled	Actual	Comment	Reference
P	539	HIS	-	expression tag	UNP O33245
P	540	HIS	-	expression tag	UNP O33245
R	301	OZT	-	amidation	UNP O33245
R	535	HIS	-	expression tag	UNP O33245
R	536	HIS	-	expression tag	UNP O33245
R	537	HIS	-	expression tag	UNP O33245
R	538	HIS	-	expression tag	UNP O33245
R	539	HIS	-	expression tag	UNP O33245
R	540	HIS	-	expression tag	UNP O33245
T	301	OZT	-	amidation	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
X	301	OZT	-	amidation	UNP O33245
X	535	HIS	-	expression tag	UNP O33245
X	536	HIS	-	expression tag	UNP O33245
X	537	HIS	-	expression tag	UNP O33245
X	538	HIS	-	expression tag	UNP O33245
X	539	HIS	-	expression tag	UNP O33245
X	540	HIS	-	expression tag	UNP O33245
Z	301	OZT	-	amidation	UNP O33245
Z	535	HIS	-	expression tag	UNP O33245
Z	536	HIS	-	expression tag	UNP O33245
Z	537	HIS	-	expression tag	UNP O33245
Z	538	HIS	-	expression tag	UNP O33245
Z	539	HIS	-	expression tag	UNP O33245
Z	540	HIS	-	expression tag	UNP O33245
2	301	OZT	-	amidation	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 subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	G	222	1638	1027	282	324	5	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	V	224	1647	1032	284	326	5	0	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	535	HIS	-	expression tag	UNP O33245
G	536	HIS	-	expression tag	UNP O33245
G	537	HIS	-	expression tag	UNP O33245
G	538	HIS	-	expression tag	UNP O33245
G	539	HIS	-	expression tag	UNP O33245
G	540	HIS	-	expression tag	UNP O33245
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

- Molecule 3 is a protein called Proteasome subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	D	213	1643	1028	301	311	3	0	0	0
3	A	214	1651	1033	302	312	4	0	0	0
3	B	216	1662	1040	304	314	4	0	0	0
3	F	212	1634	1023	300	308	3	0	0	0
3	I	217	1670	1046	305	315	4	0	0	0
3	K	216	1662	1041	304	314	3	0	0	0
3	M	194	1489	935	268	284	2	0	0	0
3	O	214	1650	1033	302	312	3	0	0	0
3	Q	213	1643	1028	301	311	3	0	0	0
3	S	215	1658	1038	303	313	4	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	U	212	Total	C	N	O	S	0	0	0
			1637	1025	300	309	3			
3	W	209	Total	C	N	O	S	0	0	0
			1612	1010	296	304	2			
3	Y	213	Total	C	N	O	S	0	0	0
			1643	1028	301	311	3			
3	1	213	Total	C	N	O	S	0	0	0
			1643	1028	301	311	3			

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	-	initiating methionine	UNP O33244
S	9	MET	-	initiating methionine	UNP O33244
U	9	MET	-	initiating methionine	UNP O33244
W	9	MET	-	initiating methionine	UNP O33244
Y	9	MET	-	initiating methionine	UNP O33244
1	9	MET	-	initiating methionine	UNP O33244

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	H	42	Total	O	0	0
			42	42		
4	C	33	Total	O	0	0
			33	33		
4	E	38	Total	O	0	0
			38	38		
4	G	41	Total	O	0	0
			41	41		
4	J	33	Total	O	0	0
			33	33		
4	L	43	Total	O	0	0
			43	43		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	N	74	Total O 74 74	0	0
4	P	68	Total O 68 68	0	0
4	R	41	Total O 41 41	0	0
4	T	34	Total O 34 34	0	0
4	V	70	Total O 70 70	0	0
4	X	51	Total O 51 51	0	0
4	Z	35	Total O 35 35	0	0
4	2	45	Total O 45 45	0	0
4	D	18	Total O 18 18	0	0
4	A	36	Total O 36 36	0	0
4	B	46	Total O 46 46	0	0
4	F	33	Total O 33 33	0	0
4	I	39	Total O 39 39	0	0
4	K	30	Total O 30 30	0	0
4	M	19	Total O 19 19	0	0
4	O	33	Total O 33 33	0	0
4	Q	13	Total O 13 13	0	0
4	S	19	Total O 19 19	0	0
4	U	31	Total O 31 31	0	0
4	W	18	Total O 18 18	0	0
4	Y	23	Total O 23 23	0	0

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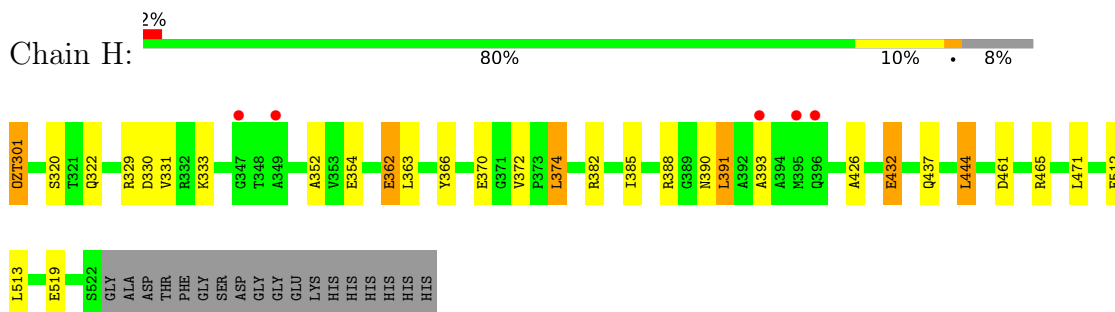
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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
4	1	22	Total	O	0	0
			22	22		

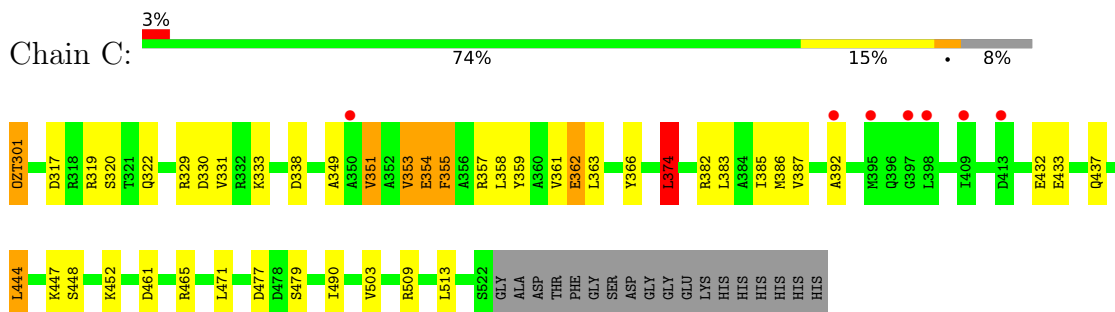
### 3 Residue-property plots [i](#)

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

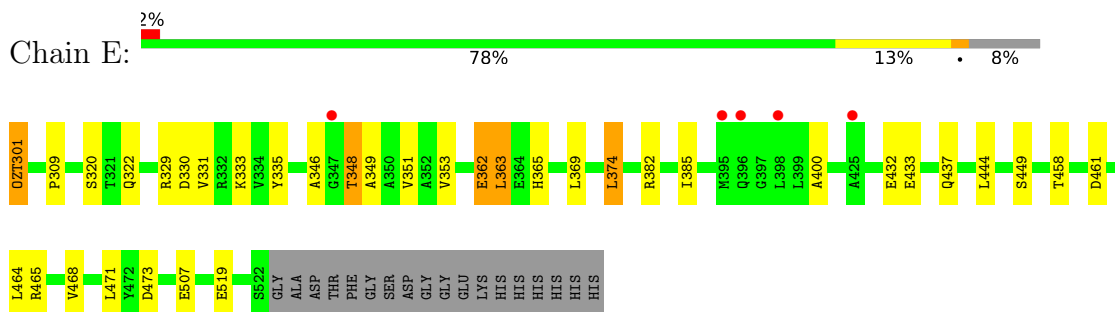
- Molecule 1: Proteasome subunit beta



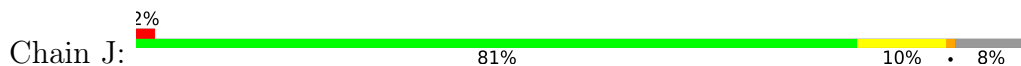
- Molecule 1: Proteasome subunit beta

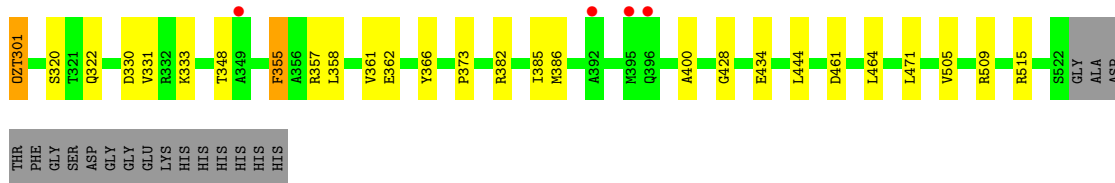


- Molecule 1: Proteasome subunit beta

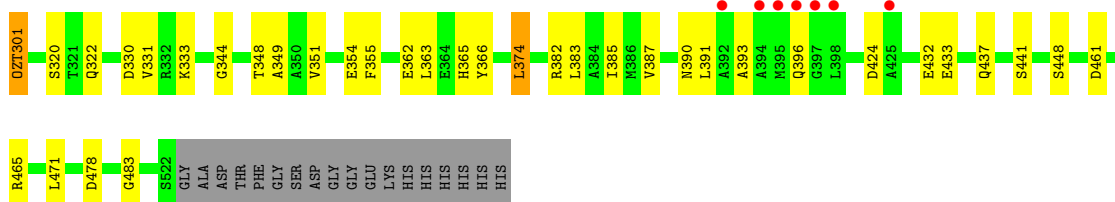
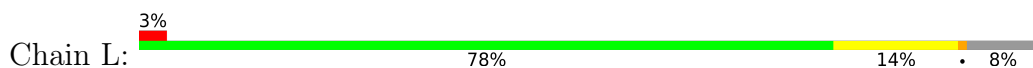


- Molecule 1: Proteasome subunit beta

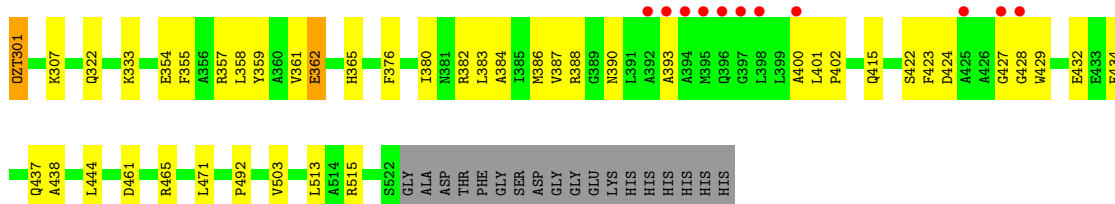
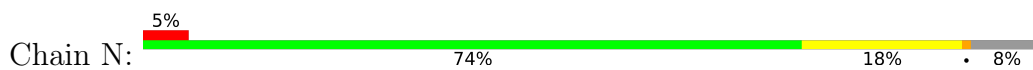




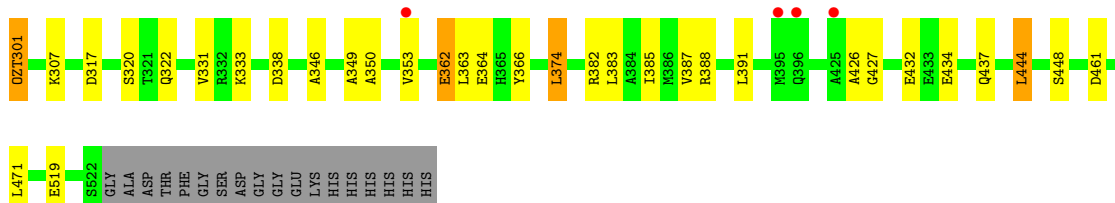
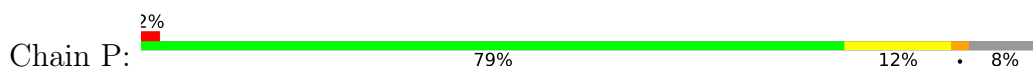
• Molecule 1: Proteasome subunit beta



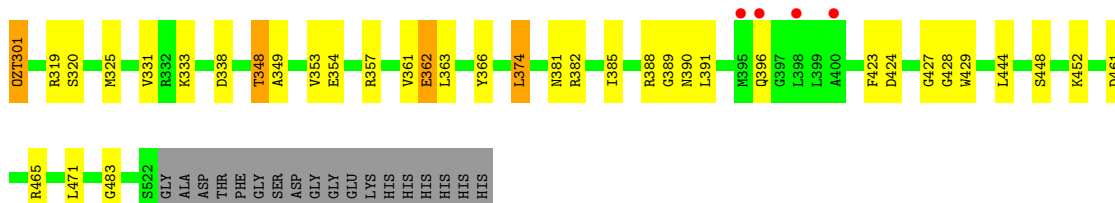
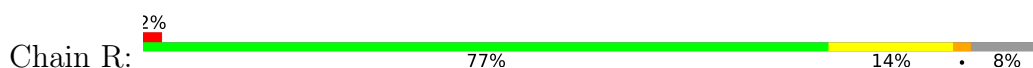
• Molecule 1: Proteasome subunit beta



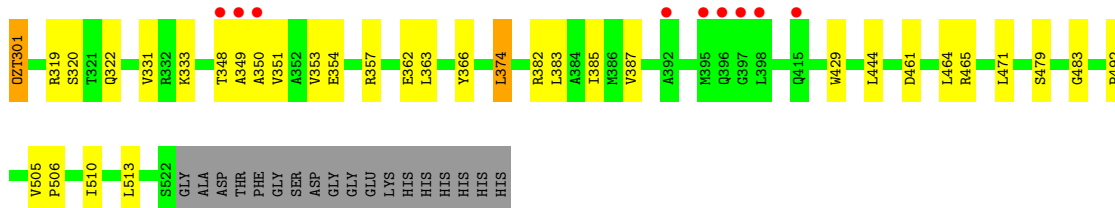
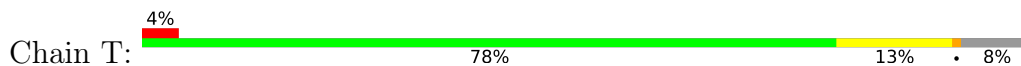
• Molecule 1: Proteasome subunit beta



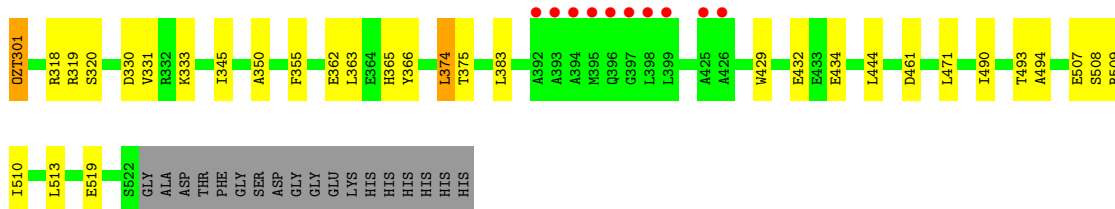
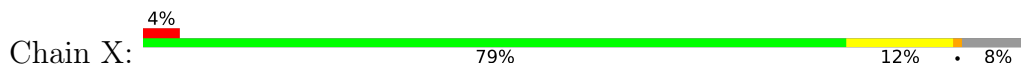
• Molecule 1: Proteasome subunit beta



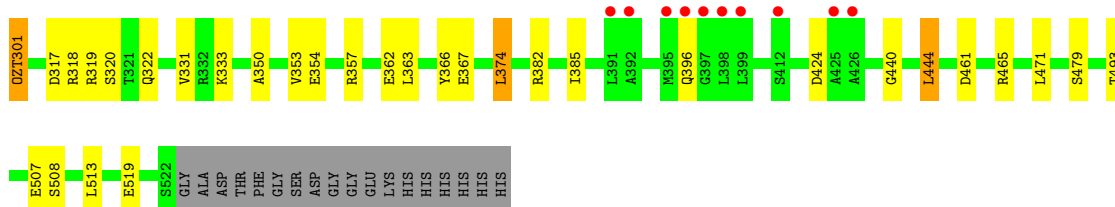
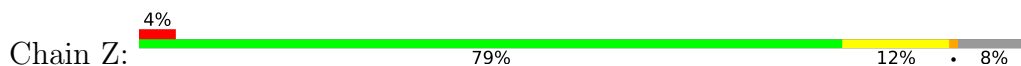
• Molecule 1: Proteasome subunit beta



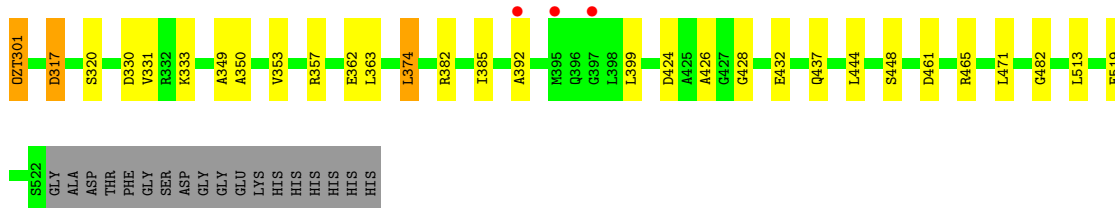
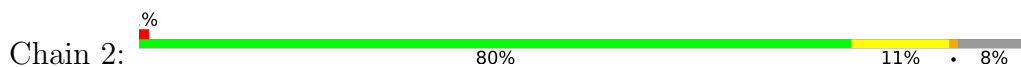
• Molecule 1: Proteasome subunit beta



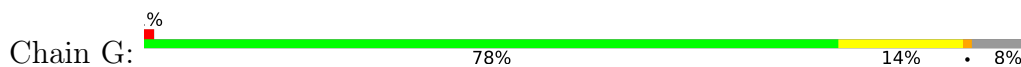
• Molecule 1: Proteasome subunit beta

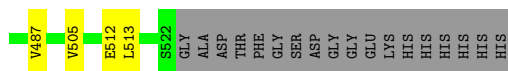


• Molecule 1: Proteasome subunit beta

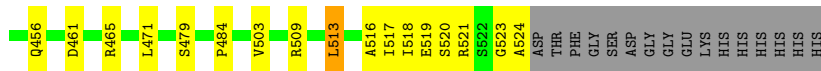


• Molecule 2: Proteasome subunit beta

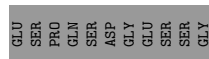
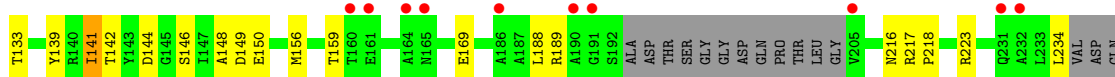




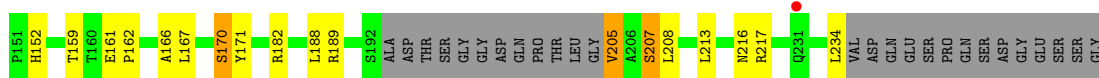
• Molecule 2: Proteasome subunit beta



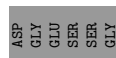
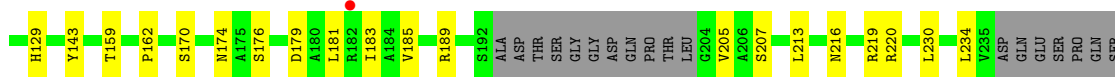
• Molecule 3: Proteasome subunit alpha



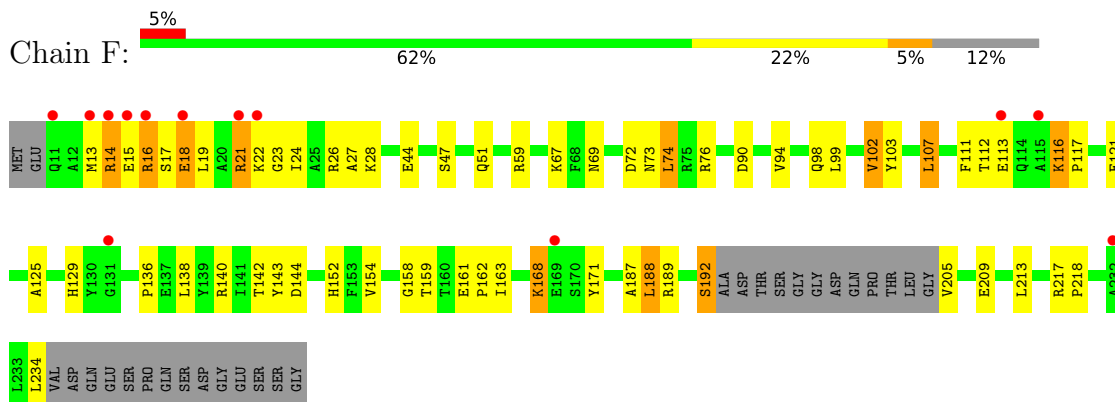
• Molecule 3: Proteasome subunit alpha



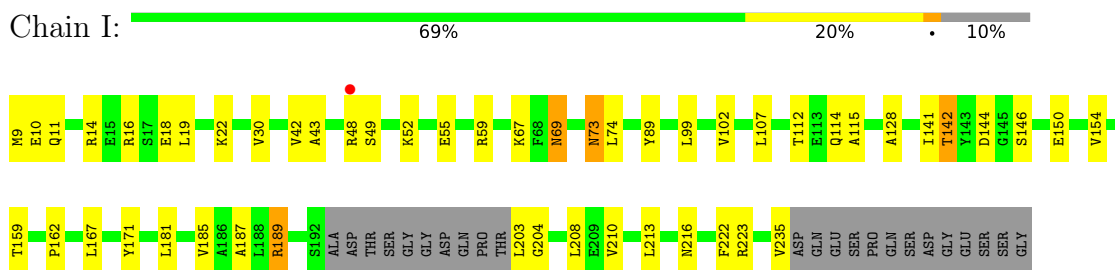
• Molecule 3: Proteasome subunit alpha



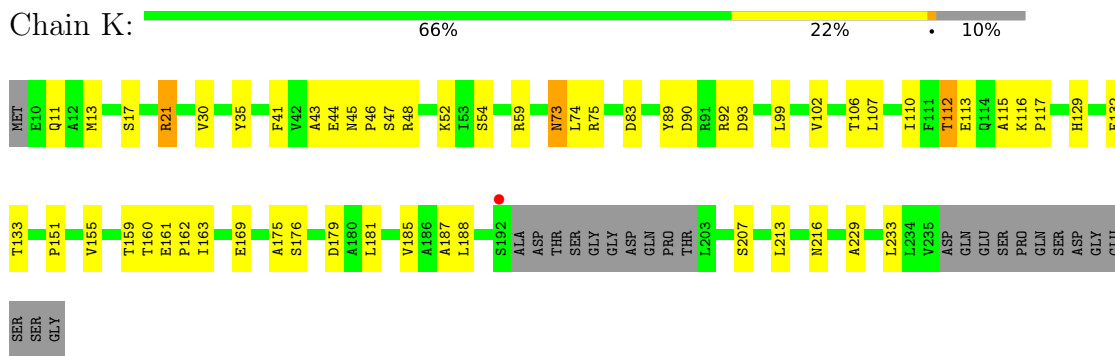
- Molecule 3: Proteasome subunit alpha



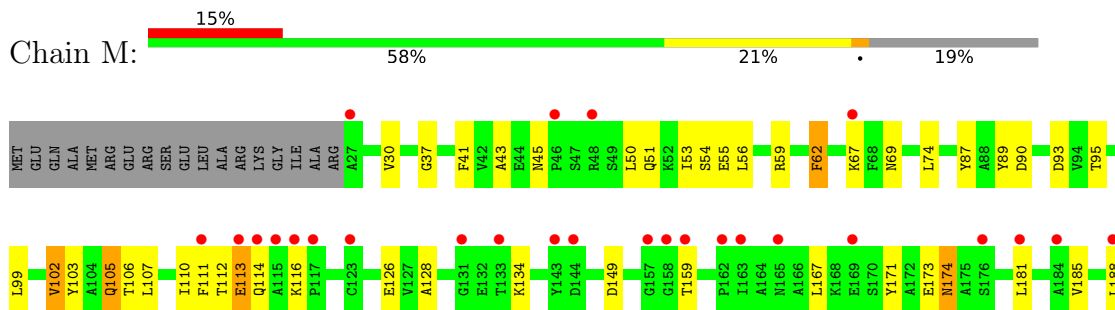
- Molecule 3: Proteasome subunit alpha



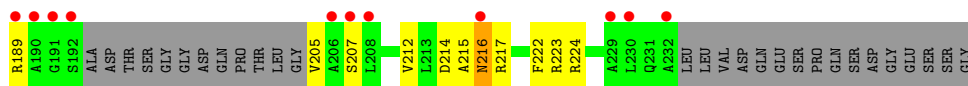
- Molecule 3: Proteasome subunit alpha



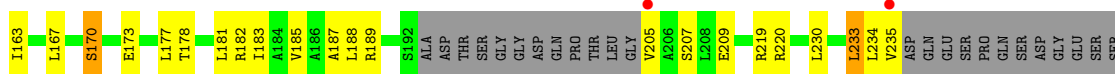
- Molecule 3: Proteasome subunit alpha





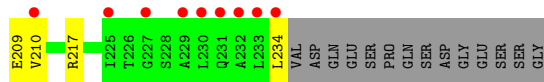
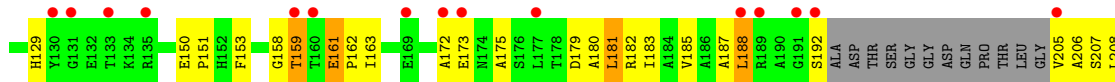
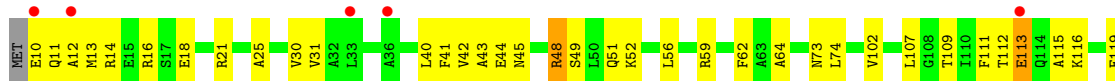


• Molecule 3: Proteasome subunit alpha



GLY

• Molecule 3: Proteasome subunit alpha

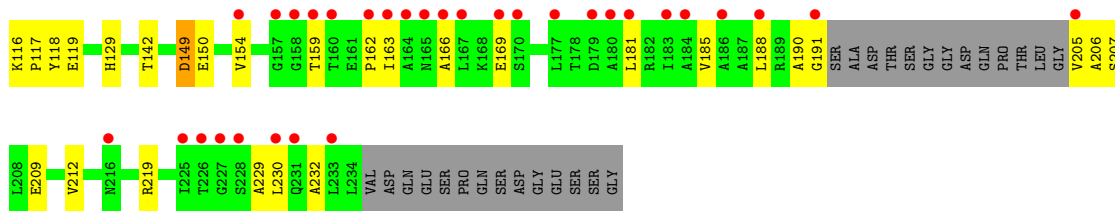


• Molecule 3: Proteasome subunit alpha

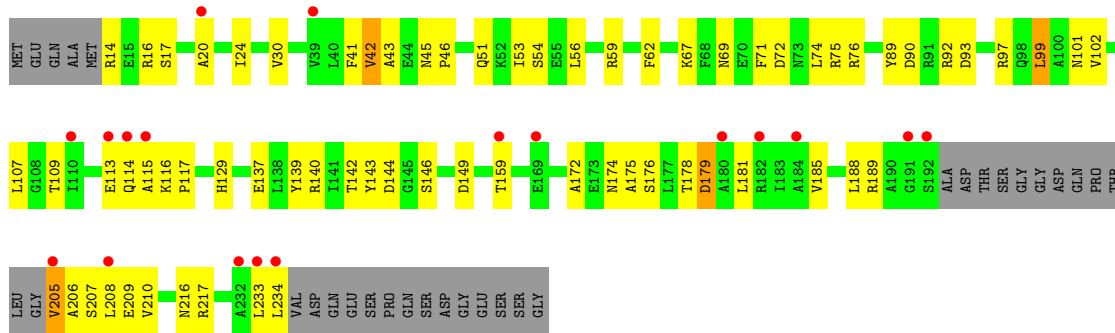


• Molecule 3: Proteasome subunit alpha

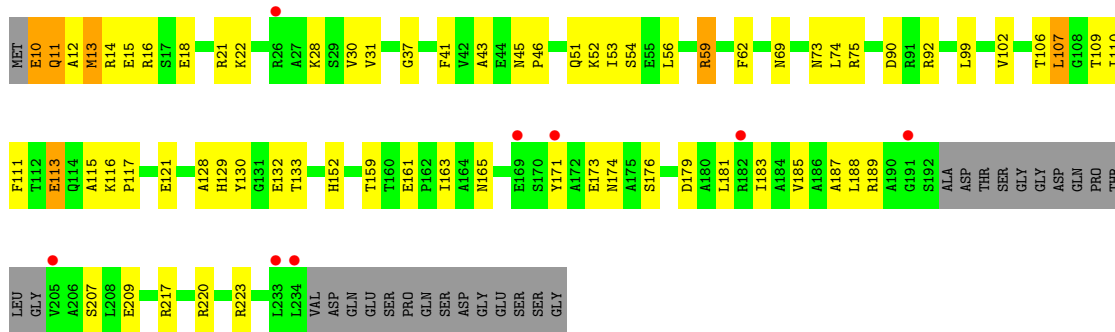




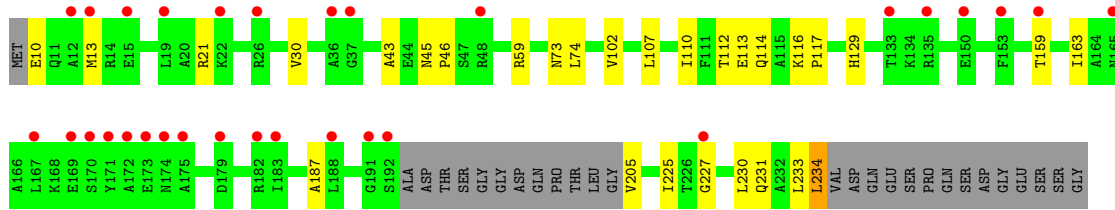
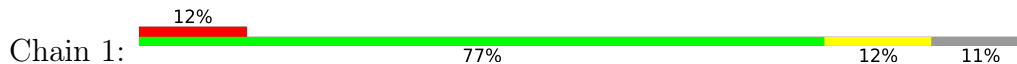
• Molecule 3: Proteasome subunit alpha



• Molecule 3: Proteasome subunit alpha



• Molecule 3: Proteasome subunit alpha



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	118.97Å 207.55Å 142.28Å 90.00° 102.42° 90.00°	Depositor
Resolution (Å)	29.87 – 2.60 34.93 – 2.57	Depositor EDS
% Data completeness (in resolution range)	96.5 (29.87-2.60) 95.2 (34.93-2.57)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.90 (at 2.57Å)	Xtrriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.224 , 0.257 0.220 , 0.249	Depositor DCC
$R_{free}$ test set	10154 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	38.0	Xtrriage
Anisotropy	0.235	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 49.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	46890	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	53.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.13% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality i

### 5.1 Standard geometry i

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	2	0.77	0/1655	0.85	1/2244 (0.0%)
1	C	0.70	0/1655	0.77	2/2244 (0.1%)
1	E	0.73	0/1655	0.77	1/2244 (0.0%)
1	H	0.76	1/1655 (0.1%)	0.79	0/2244
1	J	0.73	0/1655	0.81	0/2244
1	L	0.74	0/1655	0.82	0/2244
1	N	0.82	0/1655	0.80	0/2244
1	P	0.83	0/1655	0.77	1/2244 (0.0%)
1	R	0.72	0/1655	0.75	1/2244 (0.0%)
1	T	0.80	0/1655	0.81	0/2244
1	X	0.79	0/1655	0.80	0/2244
1	Z	0.73	0/1655	0.82	0/2244
2	G	0.70	0/1662	0.81	1/2254 (0.0%)
2	V	0.79	0/1671	0.76	1/2266 (0.0%)
3	1	0.76	0/1667	0.86	0/2251
3	A	0.76	0/1675	0.80	2/2261 (0.1%)
3	B	0.77	0/1686	0.79	1/2276 (0.0%)
3	D	0.70	0/1667	0.79	1/2251 (0.0%)
3	F	0.70	0/1658	0.83	1/2239 (0.0%)
3	I	0.72	0/1694	0.76	1/2287 (0.0%)
3	K	0.69	0/1686	0.81	0/2277
3	M	0.68	0/1513	0.74	1/2048 (0.0%)
3	O	0.72	0/1674	0.79	1/2261 (0.0%)
3	Q	0.71	0/1667	0.81	0/2251
3	S	0.71	0/1682	0.80	1/2271 (0.0%)
3	U	0.68	0/1661	0.78	0/2243
3	W	0.66	0/1636	0.74	1/2210 (0.0%)
3	Y	0.67	0/1667	0.73	0/2251
All	All	0.74	1/46426 (0.0%)	0.79	18/62825 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	519	GLU	CB-CG	5.14	1.61	1.52

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	213	LEU	N-CA-C	-5.80	95.33	111.00
1	P	338	ASP	CB-CG-OD1	5.59	123.33	118.30
1	E	374	LEU	CA-CB-CG	5.46	127.86	115.30
1	C	338	ASP	CB-CG-OD1	5.45	123.20	118.30
1	C	374	LEU	CA-CB-CG	5.42	127.76	115.30
1	2	374	LEU	CA-CB-CG	5.39	127.69	115.30
3	I	213	LEU	N-CA-C	-5.36	96.54	111.00
3	W	189	ARG	NE-CZ-NH1	5.35	122.97	120.30
3	B	213	LEU	N-CA-C	-5.33	96.61	111.00
2	V	338	ASP	CB-CG-OD1	5.33	123.09	118.30
3	D	189	ARG	NE-CZ-NH1	5.22	122.91	120.30
3	A	213	LEU	N-CA-C	-5.21	96.92	111.00
2	G	338	ASP	CB-CG-OD1	5.12	122.91	118.30
3	M	189	ARG	NE-CZ-NH1	5.12	122.86	120.30
3	O	189	ARG	NE-CZ-NH1	5.09	122.85	120.30
1	R	338	ASP	CB-CG-OD1	5.09	122.88	118.30
3	S	213	LEU	N-CA-C	-5.03	97.42	111.00
3	A	189	ARG	NE-CZ-NH1	5.01	122.81	120.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	2	1640	0	1630	31	0
1	C	1640	0	1630	39	0
1	E	1640	0	1630	29	0
1	H	1640	0	1630	29	0
1	J	1640	0	1630	22	0
1	L	1640	0	1630	37	0
1	N	1640	0	1630	40	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	P	1640	0	1630	34	0
1	R	1640	0	1630	36	0
1	T	1640	0	1630	39	0
1	X	1640	0	1630	31	0
1	Z	1640	0	1630	24	0
2	G	1638	0	1630	31	0
2	V	1647	0	1638	68	0
3	1	1643	0	1641	29	0
3	A	1651	0	1650	50	0
3	B	1662	0	1662	39	0
3	D	1643	0	1641	43	0
3	F	1634	0	1635	80	0
3	I	1670	0	1673	50	0
3	K	1662	0	1664	54	0
3	M	1489	0	1474	55	0
3	O	1650	0	1650	65	0
3	Q	1643	0	1641	75	0
3	S	1658	0	1659	54	0
3	U	1637	0	1636	73	0
3	W	1612	0	1613	43	0
3	Y	1643	0	1641	54	0
4	1	22	0	0	1	0
4	2	45	0	0	10	0
4	A	36	0	0	5	0
4	B	46	0	0	4	0
4	C	33	0	0	2	0
4	D	18	0	0	7	0
4	E	38	0	0	6	0
4	F	33	0	0	1	0
4	G	41	0	0	4	0
4	H	42	0	0	5	0
4	I	39	0	0	4	0
4	J	33	0	0	5	0
4	K	30	0	0	5	0
4	L	43	0	0	4	0
4	M	19	0	0	4	0
4	N	74	0	0	4	0
4	O	33	0	0	4	0
4	P	68	0	0	6	0
4	Q	13	0	0	2	0
4	R	41	0	0	6	0
4	S	19	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	T	34	0	0	2	0
4	U	31	0	0	9	0
4	V	70	0	0	4	0
4	W	18	0	0	0	0
4	X	51	0	0	3	0
4	Y	23	0	0	4	0
4	Z	35	0	0	2	0
All	All	46890	0	45708	1148	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 13.

All (1148) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:301:OZT:H17	1:2:333:LYS:NZ	1.32	1.39
2:V:348:THR:HG22	2:V:351:VAL:CG2	1.58	1.33
3:U:163:ILE:CG1	3:U:191:GLY:HA3	1.65	1.27
3:Q:181:LEU:C	3:Q:181:LEU:HD12	1.55	1.24
1:C:349:ALA:O	1:C:353:VAL:HG22	1.38	1.24
3:Q:180:ALA:HA	3:Q:183:ILE:HD12	1.22	1.21
3:Q:18:GLU:CD	3:Q:21:ARG:HH12	1.45	1.19
1:C:301:OZT:H17	1:C:333:LYS:NZ	1.57	1.19
3:F:16:ARG:HB3	3:F:16:ARG:NH1	1.55	1.18
3:1:231:GLN:HA	3:1:234:LEU:CD1	1.75	1.17
1:H:391:LEU:HD12	1:H:391:LEU:O	1.45	1.16
2:V:348:THR:CG2	2:V:351:VAL:CG2	2.24	1.16
3:D:217:ARG:NH1	3:D:223:ARG:HD3	1.60	1.13
3:F:21:ARG:HD2	3:F:21:ARG:O	1.49	1.13
1:T:301:OZT:H17	1:T:333:LYS:NZ	1.64	1.12
3:K:52:LYS:HD2	4:K:942:HOH:O	1.47	1.11
2:V:484:PRO:HG2	2:V:518:ILE:HD11	1.31	1.11
3:W:205:VAL:HG23	3:W:207:SER:H	0.99	1.11
1:X:301:OZT:H17	1:X:333:LYS:NZ	1.66	1.11
1:C:301:OZT:H17	1:C:333:LYS:HZ3	0.94	1.10
3:1:231:GLN:HA	3:1:234:LEU:HD11	1.32	1.10
3:S:205:VAL:HG22	3:S:206:ALA:N	1.56	1.10
3:U:163:ILE:HG13	3:U:191:GLY:HA3	1.10	1.09
3:A:137:GLU:HB3	3:O:48:ARG:NH2	1.65	1.09
2:V:348:THR:O	2:V:351:VAL:HG22	1.52	1.09
3:F:168:LYS:HB2	3:F:168:LYS:NZ	1.49	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:21:ARG:HG2	3:F:21:ARG:HH11	0.98	1.08
3:F:168:LYS:HB2	3:F:168:LYS:HZ3	0.92	1.08
1:2:301:OZT:C7	1:2:333:LYS:HZ3	1.65	1.08
3:Q:205:VAL:HG13	3:Q:206:ALA:N	1.67	1.06
3:Q:205:VAL:HG13	3:Q:206:ALA:H	1.12	1.06
3:S:205:VAL:CG2	3:S:206:ALA:H	1.62	1.05
2:V:348:THR:CG2	2:V:351:VAL:HG21	1.87	1.03
3:Q:181:LEU:HD12	3:Q:181:LEU:O	1.55	1.03
3:Q:179:ASP:O	3:Q:183:ILE:HG13	1.58	1.03
2:V:348:THR:CG2	2:V:351:VAL:HG22	1.88	1.02
1:C:301:OZT:C7	1:C:333:LYS:HZ3	1.73	1.02
3:U:31:VAL:HB	3:U:42:VAL:HG12	1.43	1.01
2:V:348:THR:HG22	2:V:351:VAL:HG22	1.03	1.01
3:F:16:ARG:HB3	3:F:16:ARG:HH11	0.83	1.00
3:U:166:ALA:HB1	4:U:959:HOH:O	1.59	1.00
3:1:231:GLN:O	3:1:234:LEU:HD12	1.61	1.00
1:R:301:OZT:H17	1:R:333:LYS:NZ	1.77	0.99
3:I:235:VAL:HG12	3:I:235:VAL:O	1.60	0.99
3:F:16:ARG:HH11	3:F:16:ARG:CB	1.75	0.99
3:Q:30:VAL:HG13	3:Q:43:ALA:HB2	1.42	0.99
3:S:112:THR:HG22	3:S:113:GLU:HG3	1.43	0.99
3:B:181:LEU:O	3:B:185:VAL:HG23	1.63	0.98
3:O:205:VAL:HG12	3:O:205:VAL:O	1.62	0.98
3:Q:205:VAL:CG1	3:Q:206:ALA:H	1.75	0.98
1:J:428:GLY:HA3	1:T:350:ALA:CB	1.92	0.97
3:1:231:GLN:CA	3:1:234:LEU:CD1	2.41	0.97
3:F:159:THR:HG22	3:F:162:PRO:HD2	1.46	0.96
3:O:159:THR:HG22	3:O:162:PRO:CD	1.95	0.96
3:A:137:GLU:HB3	3:O:48:ARG:HH22	1.21	0.96
3:D:217:ARG:HH12	3:D:223:ARG:HD3	1.30	0.95
3:Q:181:LEU:C	3:Q:181:LEU:CD1	2.31	0.95
3:W:205:VAL:HG23	3:W:207:SER:N	1.80	0.95
3:S:205:VAL:HG22	3:S:206:ALA:H	0.79	0.95
3:F:16:ARG:NH1	3:F:16:ARG:CB	2.30	0.95
1:L:382:ARG:NH2	1:L:385:ILE:CD1	2.30	0.94
3:F:51:GLN:HG2	3:F:209:GLU:OE2	1.65	0.94
3:A:137:GLU:CG	3:O:48:ARG:NH2	2.30	0.94
1:H:301:OZT:H17	1:H:333:LYS:NZ	1.84	0.93
1:T:301:OZT:H17	1:T:333:LYS:HZ3	1.26	0.93
3:A:137:GLU:CB	3:O:48:ARG:NH2	2.30	0.93
3:S:233:LEU:HD12	3:S:233:LEU:N	1.84	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:1:231:GLN:CA	3:1:234:LEU:HD11	1.97	0.93
1:Z:301:OZT:H17	1:Z:333:LYS:NZ	1.84	0.93
3:O:159:THR:HG22	3:O:162:PRO:HD2	1.50	0.93
1:2:301:OZT:C7	1:2:333:LYS:NZ	2.24	0.92
3:F:21:ARG:HG2	3:F:21:ARG:NH1	1.77	0.92
3:S:233:LEU:HD12	3:S:233:LEU:H	1.35	0.91
1:X:301:OZT:H17	1:X:333:LYS:HZ3	1.31	0.91
2:V:362:GLU:OE2	2:V:382:ARG:HD3	1.70	0.91
1:X:301:OZT:C7	1:X:333:LYS:NZ	2.34	0.90
3:M:112:THR:HG22	3:M:113:GLU:OE1	1.72	0.89
3:D:114:GLN:HE21	3:D:114:GLN:HA	1.37	0.89
3:F:168:LYS:HZ3	3:F:168:LYS:CB	1.82	0.89
3:O:18:GLU:HG3	3:O:22:LYS:HE3	1.53	0.89
3:D:217:ARG:HH12	3:D:223:ARG:HB2	1.38	0.88
1:C:301:OZT:C7	1:C:333:LYS:NZ	2.33	0.88
1:X:301:OZT:C7	1:X:333:LYS:HZ3	1.84	0.88
3:K:44:GLU:HG2	4:K:984:HOH:O	1.72	0.88
1:R:301:OZT:H17	1:R:333:LYS:HZ3	1.37	0.88
3:O:112:THR:CG2	3:U:115:ALA:HB3	2.03	0.87
3:U:31:VAL:HB	3:U:42:VAL:CG1	2.04	0.87
3:F:168:LYS:NZ	3:F:168:LYS:CB	2.30	0.87
3:U:163:ILE:HG13	3:U:191:GLY:CA	2.01	0.86
1:L:382:ARG:NH2	1:L:385:ILE:HD13	1.89	0.86
3:W:42:VAL:HG13	3:W:210:VAL:HG22	1.57	0.86
1:P:301:OZT:H27	1:P:333:LYS:NZ	1.91	0.86
1:X:355:PHE:CZ	1:X:383:LEU:HD11	2.10	0.86
3:I:159:THR:O	3:I:162:PRO:HD2	1.75	0.86
3:O:235:VAL:HG12	3:O:235:VAL:O	1.75	0.85
1:L:301:OZT:H17	1:L:333:LYS:NZ	1.92	0.85
3:A:137:GLU:CG	3:O:48:ARG:HH21	1.88	0.85
3:Y:13:MET:HA	3:Y:13:MET:CE	2.06	0.85
1:P:349:ALA:O	1:P:353:VAL:HG23	1.76	0.85
3:U:114:GLN:HE22	3:U:118:TYR:HE1	1.21	0.85
1:L:391:LEU:O	1:L:391:LEU:HD12	1.77	0.85
3:U:111:PHE:CD2	3:U:111:PHE:O	2.30	0.85
3:A:137:GLU:CD	3:O:48:ARG:HH21	1.80	0.85
3:D:18:GLU:HB2	4:D:743:HOH:O	1.78	0.84
3:1:234:LEU:HD12	3:1:234:LEU:H	1.41	0.84
3:Q:48:ARG:HD2	3:Q:49:SER:H	1.42	0.84
1:J:428:GLY:CA	1:T:350:ALA:HB1	2.07	0.84
3:A:159:THR:HG22	3:A:162:PRO:CD	2.08	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:U:163:ILE:CG1	3:U:191:GLY:CA	2.54	0.84
3:Q:180:ALA:HA	3:Q:183:ILE:CD1	2.06	0.83
3:B:15:GLU:HG3	4:B:855:HOH:O	1.78	0.83
1:T:301:OZT:H17	1:T:333:LYS:HZ1	1.42	0.83
3:1:230:LEU:O	3:1:234:LEU:HD11	1.78	0.83
1:H:432:GLU:HG3	4:H:541:HOH:O	1.77	0.83
1:2:301:OZT:H17	1:2:333:LYS:HZ1	1.38	0.83
2:V:348:THR:O	2:V:351:VAL:CG2	2.26	0.82
1:H:352:ALA:HB1	4:H:832:HOH:O	1.79	0.82
2:V:517:ILE:O	2:V:521:ARG:HG3	1.79	0.82
3:1:231:GLN:C	3:1:234:LEU:HD12	1.99	0.82
3:Q:48:ARG:CD	3:Q:49:SER:H	1.92	0.82
2:V:348:THR:HG21	2:V:351:VAL:HG21	1.60	0.81
3:D:103:TYR:O	3:D:107:LEU:HD23	1.79	0.81
1:Z:301:OZT:H17	1:Z:333:LYS:HZ3	1.42	0.81
3:I:19:LEU:HD22	3:S:9:MET:HE3	1.60	0.81
1:P:301:OZT:C7	1:P:333:LYS:NZ	2.43	0.81
1:J:301:OZT:H17	1:J:333:LYS:NZ	1.95	0.81
3:F:21:ARG:HD2	3:F:21:ARG:C	2.01	0.81
1:P:301:OZT:H27	1:P:333:LYS:HZ1	1.46	0.80
3:I:142:THR:HG23	3:I:144:ASP:OD1	1.82	0.80
3:D:114:GLN:HA	3:D:114:GLN:NE2	1.93	0.80
3:I:235:VAL:O	3:I:235:VAL:CG1	2.30	0.80
3:O:205:VAL:O	3:O:205:VAL:CG1	2.30	0.80
1:J:428:GLY:CA	1:T:350:ALA:CB	2.60	0.80
3:F:21:ARG:HH11	3:F:21:ARG:CG	1.85	0.80
3:I:142:THR:CG2	3:I:144:ASP:OD1	2.30	0.80
1:H:391:LEU:HD12	1:H:391:LEU:C	2.01	0.80
3:Q:181:LEU:O	3:Q:181:LEU:CD1	2.30	0.80
1:R:391:LEU:HD12	1:R:391:LEU:O	1.82	0.79
3:D:150:GLU:HG2	4:D:603:HOH:O	1.81	0.79
3:F:24:ILE:O	3:F:24:ILE:CG2	2.30	0.79
3:Y:181:LEU:O	3:Y:185:VAL:HG23	1.82	0.79
1:H:382:ARG:HH21	1:H:385:ILE:HD12	1.47	0.79
3:Y:18:GLU:O	3:Y:22:LYS:HG3	1.83	0.79
3:F:159:THR:HG22	3:F:162:PRO:CD	2.12	0.79
3:1:231:GLN:O	3:1:234:LEU:CD1	2.30	0.79
1:H:382:ARG:HH21	1:H:385:ILE:CD1	1.95	0.79
1:N:355:PHE:HE2	1:N:383:LEU:HD11	1.47	0.79
3:U:162:PRO:HB2	3:U:191:GLY:HA2	1.64	0.79
3:1:230:LEU:O	3:1:234:LEU:CD1	2.30	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:179:ASP:O	3:Q:183:ILE:CG1	2.30	0.78
1:X:301:OZT:H17	1:X:333:LYS:HZ1	1.45	0.78
3:O:178:THR:HG23	3:O:233:LEU:O	1.83	0.78
3:O:205:VAL:HG22	3:O:230:LEU:HG	1.65	0.78
3:Q:18:GLU:CD	3:Q:21:ARG:NH1	2.31	0.78
3:W:20:ALA:O	3:W:24:ILE:HG13	1.84	0.78
3:D:30:VAL:HG13	3:D:43:ALA:HB2	1.66	0.78
1:P:444:LEU:HB3	4:P:568:HOH:O	1.84	0.78
1:2:482:GLY:HA3	4:2:683:HOH:O	1.84	0.78
3:F:159:THR:CG2	3:F:162:PRO:HD2	2.12	0.77
3:A:137:GLU:HG2	3:O:48:ARG:NH2	2.00	0.77
3:S:233:LEU:H	3:S:233:LEU:CD1	1.97	0.77
1:X:330:ASP:OD1	1:X:490:ILE:HD13	1.85	0.77
1:P:382:ARG:HH21	1:P:385:ILE:CD1	1.98	0.77
3:1:231:GLN:HA	3:1:234:LEU:HD13	1.67	0.77
3:1:225:ILE:HG21	3:1:233:LEU:CD1	2.15	0.76
1:R:390:ASN:HB2	4:R:680:HOH:O	1.85	0.76
3:U:16:ARG:HH12	3:U:111:PHE:C	1.87	0.76
1:N:301:OZT:H17	1:N:333:LYS:NZ	2.00	0.76
1:E:346:ALA:HA	4:E:876:HOH:O	1.85	0.76
3:U:205:VAL:HG12	3:U:206:ALA:N	2.01	0.76
2:G:388:ARG:HD3	4:G:697:HOH:O	1.85	0.76
3:Q:48:ARG:HD2	3:Q:48:ARG:N	1.99	0.76
3:U:106:THR:O	3:U:110:ILE:HG13	1.85	0.75
3:S:90:ASP:HB3	3:S:93:ASP:OD2	1.86	0.75
3:K:151:PRO:HD2	4:K:255:HOH:O	1.87	0.75
3:A:159:THR:HG22	3:A:162:PRO:HD2	1.67	0.75
1:N:390:ASN:ND2	1:N:393:ALA:HB3	2.02	0.74
2:V:484:PRO:CG	2:V:518:ILE:HD11	2.15	0.74
3:D:217:ARG:NH1	3:D:223:ARG:HB2	2.01	0.74
2:G:487:VAL:HG13	2:V:521:ARG:HB3	1.68	0.74
3:B:20:ALA:O	3:B:24:ILE:HG13	1.86	0.74
1:H:301:OZT:H17	1:H:333:LYS:HZ3	1.49	0.74
1:H:390:ASN:ND2	1:H:393:ALA:HB3	2.03	0.74
1:C:354:GLU:OE2	1:C:355:PHE:HA	1.88	0.74
3:1:231:GLN:C	3:1:234:LEU:CD1	2.55	0.74
3:K:47:SER:OG	3:M:149:ASP:CB	2.36	0.74
3:S:169:GLU:HA	3:S:169:GLU:OE1	1.88	0.74
3:Y:133:THR:O	3:Y:133:THR:HG23	1.86	0.73
3:M:41:PHE:HB3	3:M:53:ILE:HD13	1.69	0.73
3:D:59:ARG:NH2	3:D:217:ARG:O	2.20	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:W:51:GLN:HG2	3:W:209:GLU:OE2	1.88	0.73
2:G:345:ILE:N	2:G:345:ILE:HD12	2.04	0.73
3:A:92:ARG:HH11	3:A:92:ARG:HB3	1.53	0.73
1:T:301:OZT:C7	1:T:333:LYS:NZ	2.47	0.72
1:2:301:OZT:H17	1:2:333:LYS:HZ3	0.78	0.72
1:E:301:OZT:H2	4:E:876:HOH:O	1.89	0.72
3:A:33:LEU:N	3:A:33:LEU:HD23	2.05	0.72
3:S:161:GLU:CD	3:S:161:GLU:H	1.92	0.72
3:W:92:ARG:HH11	3:W:92:ARG:HB3	1.54	0.72
3:Q:159:THR:O	3:Q:163:ILE:HD12	1.89	0.72
1:X:366:TYR:CE2	1:X:374:LEU:HD13	2.24	0.72
3:Y:51:GLN:HG2	3:Y:209:GLU:OE2	1.89	0.71
3:M:67:LYS:HE2	3:M:69:ASN:HD21	1.54	0.71
2:V:465:ARG:HG3	2:V:513:LEU:HD11	1.70	0.71
3:M:51:GLN:OE1	3:M:224:ARG:NH2	2.24	0.71
1:N:384:ALA:O	1:N:388:ARG:HG3	1.90	0.71
3:U:31:VAL:HG23	3:U:188:LEU:HD21	1.72	0.71
1:C:349:ALA:O	1:C:353:VAL:CG2	2.30	0.71
1:J:428:GLY:HA3	1:T:350:ALA:HB3	1.72	0.71
3:W:90:ASP:HB3	3:W:93:ASP:OD2	1.91	0.71
1:J:355:PHE:HE1	4:J:546:HOH:O	1.73	0.70
3:O:182:ARG:NH2	3:O:235:VAL:HA	2.04	0.70
3:D:112:THR:CG2	3:Q:115:ALA:HB3	2.21	0.70
3:F:159:THR:CG2	3:F:162:PRO:CD	2.69	0.70
3:U:14:ARG:HG2	4:U:365:HOH:O	1.90	0.70
3:F:116:LYS:HE2	3:F:117:PRO:O	1.90	0.70
1:P:382:ARG:HH21	1:P:385:ILE:HD12	1.54	0.70
1:P:388:ARG:HG3	1:P:427:GLY:HA3	1.73	0.70
3:D:103:TYR:O	3:D:107:LEU:CD2	2.39	0.70
1:P:301:OZT:C7	1:P:333:LYS:HZ1	2.04	0.70
1:2:331:VAL:HG13	1:2:349:ALA:HB2	1.73	0.70
3:I:19:LEU:HD22	3:S:9:MET:CE	2.21	0.70
3:U:42:VAL:HG13	3:U:42:VAL:O	1.90	0.70
1:J:355:PHE:CE1	4:J:546:HOH:O	2.45	0.69
3:F:112:THR:HG21	3:M:116:LYS:HB3	1.72	0.69
3:K:44:GLU:CG	4:K:984:HOH:O	2.35	0.69
1:L:382:ARG:HD2	3:M:89:TYR:HE1	1.57	0.69
3:D:114:GLN:HE21	3:D:114:GLN:CA	2.05	0.69
3:Y:37:GLY:HA3	4:Y:725:HOH:O	1.91	0.69
3:A:92:ARG:HB3	3:A:92:ARG:NH1	2.07	0.69
3:B:116:LYS:NZ	3:B:119:GLU:OE1	2.24	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:U:149:ASP:OD1	3:U:149:ASP:C	2.30	0.69
3:W:41:PHE:HB3	3:W:53:ILE:HD13	1.75	0.69
1:C:362:GLU:OE2	1:C:382:ARG:HD3	1.92	0.69
1:C:354:GLU:OE2	1:C:354:GLU:C	2.30	0.69
3:D:117:PRO:CG	4:D:930:HOH:O	2.39	0.69
3:I:204:GLY:O	3:I:208:LEU:HG	1.91	0.69
3:S:205:VAL:CG2	3:S:206:ALA:N	2.32	0.69
3:U:42:VAL:CG1	3:U:42:VAL:O	2.40	0.69
1:H:329:ARG:HD3	4:H:948:HOH:O	1.90	0.69
3:U:16:ARG:O	3:U:117:PRO:HG2	1.93	0.69
2:V:523:GLY:O	2:V:524:ALA:C	2.32	0.69
3:F:152:HIS:HB3	3:F:171:TYR:CE2	2.28	0.69
3:A:150:GLU:HA	3:A:150:GLU:OE2	1.92	0.69
3:Q:31:VAL:N	3:Q:42:VAL:O	2.22	0.69
1:L:448:SER:HB3	1:P:448:SER:HB3	1.73	0.68
1:P:301:OZT:C7	1:P:333:LYS:HZ3	2.07	0.68
1:L:382:ARG:HH21	1:L:385:ILE:CD1	2.06	0.68
1:Z:367:GLU:OE2	3:Y:220:ARG:NH1	2.24	0.68
3:U:163:ILE:HG12	3:U:191:GLY:HA3	1.71	0.68
1:J:357:ARG:O	1:J:361:VAL:HG23	1.94	0.68
3:K:92:ARG:NH2	3:K:129:HIS:CD2	2.62	0.68
3:K:92:ARG:HH21	3:K:129:HIS:CG	2.11	0.68
3:U:52:LYS:HE3	3:U:64:ALA:O	1.94	0.68
1:T:301:OZT:C7	1:T:333:LYS:HZ3	2.04	0.68
1:J:301:OZT:H17	1:J:333:LYS:HZ3	1.58	0.68
3:D:217:ARG:HH11	3:D:223:ARG:HD3	1.58	0.67
3:K:163:ILE:HG23	3:K:187:ALA:O	1.93	0.67
3:Q:172:ALA:HB3	3:Q:175:ALA:HB2	1.76	0.67
2:V:456:GLN:CD	2:V:465:ARG:HH22	1.97	0.67
3:O:112:THR:HG22	3:U:115:ALA:HB3	1.76	0.67
3:Y:30:VAL:HG13	3:Y:43:ALA:HB2	1.77	0.67
1:R:301:OZT:H17	1:R:333:LYS:HZ1	1.58	0.67
3:B:16:ARG:NH2	3:B:114:GLN:O	2.22	0.67
3:F:112:THR:CG2	3:M:116:LYS:HB3	2.25	0.67
3:U:30:VAL:HG13	3:U:43:ALA:HB2	1.75	0.67
3:1:225:ILE:HG21	3:1:233:LEU:HD12	1.74	0.67
2:G:344:GLY:C	2:G:345:ILE:HD12	2.14	0.67
1:X:355:PHE:CZ	1:X:383:LEU:CD1	2.77	0.67
3:F:16:ARG:NH1	3:F:16:ARG:CA	2.58	0.67
3:Q:11:GLN:HA	3:Q:14:ARG:HB2	1.77	0.67
1:R:366:TYR:CE2	1:R:374:LEU:HD13	2.30	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:345:ILE:HD11	1:X:355:PHE:HD2	1.59	0.67
2:V:364:GLU:HG2	2:V:368:LYS:HE2	1.78	0.66
3:B:80:GLN:HG2	4:B:673:HOH:O	1.95	0.66
3:Y:13:MET:HA	3:Y:13:MET:HE2	1.78	0.66
1:N:359:TYR:HA	1:N:386:MET:HE1	1.77	0.66
3:F:140:ARG:HD2	3:F:154:VAL:HG13	1.76	0.66
1:L:301:OZT:H17	1:L:333:LYS:HZ3	1.59	0.66
1:L:365:HIS:ND1	3:K:83:ASP:OD2	2.25	0.66
3:U:12:ALA:O	3:U:16:ARG:HG3	1.95	0.66
1:N:307:LYS:HD3	4:N:542:HOH:O	1.96	0.66
3:D:117:PRO:HG2	4:D:930:HOH:O	1.95	0.66
3:F:16:ARG:NH1	3:F:16:ARG:C	2.49	0.66
1:L:382:ARG:NH2	1:L:385:ILE:HD12	2.09	0.66
1:R:381:ASN:O	1:R:385:ILE:HG13	1.96	0.66
2:V:484:PRO:HG2	2:V:518:ILE:CD1	2.18	0.66
3:S:161:GLU:HB2	3:S:162:PRO:CD	2.26	0.66
3:F:27:ALA:HB3	3:F:158:GLY:HA2	1.78	0.65
3:U:111:PHE:O	3:U:111:PHE:CG	2.48	0.65
3:F:24:ILE:O	3:F:24:ILE:HG23	1.94	0.65
3:Q:12:ALA:O	3:Q:16:ARG:HG3	1.95	0.65
3:I:67:LYS:HE3	4:I:428:HOH:O	1.95	0.65
3:Q:161:GLU:HB2	3:Q:162:PRO:HD3	1.79	0.65
1:C:432:GLU:OE2	1:C:437:GLN:NE2	2.30	0.65
1:R:388:ARG:NH1	1:R:427:GLY:O	2.30	0.65
2:V:382:ARG:HH21	2:V:385:ILE:CD1	2.09	0.65
3:F:16:ARG:NH1	3:F:16:ARG:O	2.30	0.65
3:Q:18:GLU:OE2	3:Q:21:ARG:NH1	2.30	0.65
3:W:179:ASP:OD1	3:W:179:ASP:N	2.30	0.65
3:B:15:GLU:OE2	3:I:9:MET:N	2.30	0.65
3:I:159:THR:HG22	3:I:162:PRO:CD	2.26	0.65
3:U:16:ARG:NH1	3:U:111:PHE:O	2.30	0.65
2:V:456:GLN:OE1	2:V:465:ARG:NH2	2.30	0.65
3:B:52:LYS:NZ	4:B:378:HOH:O	2.30	0.65
3:F:94:VAL:HA	3:F:98:GLN:HE22	1.60	0.65
3:M:59:ARG:NH2	3:M:217:ARG:O	2.30	0.65
1:E:400:ALA:HB3	4:E:551:HOH:O	1.97	0.65
1:X:432:GLU:HB3	4:X:544:HOH:O	1.97	0.65
3:A:35:TYR:CE1	3:A:37:GLY:HA3	2.32	0.65
3:I:11:GLN:OE1	3:I:14:ARG:NH1	2.30	0.65
1:T:331:VAL:CG1	1:T:349:ALA:HB1	2.27	0.64
1:X:365:HIS:NE2	4:X:550:HOH:O	2.30	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:149:ASP:OD2	3:O:48:ARG:NH1	2.30	0.64
3:B:205:VAL:HG23	3:B:234:LEU:HD12	1.79	0.64
3:F:121:GLU:OE2	3:F:140:ARG:NH1	2.30	0.64
3:W:54:SER:CB	3:W:75:ARG:HD2	2.28	0.64
3:Y:16:ARG:NH2	3:Y:111:PHE:O	2.30	0.64
2:G:412:SER:HB2	4:G:553:HOH:O	1.96	0.64
3:A:149:ASP:OD1	3:O:48:ARG:NH1	2.30	0.64
3:W:16:ARG:NH1	3:W:115:ALA:O	2.30	0.64
2:V:364:GLU:OE1	3:U:219:ARG:NH1	2.30	0.64
1:E:465:ARG:NH1	4:E:554:HOH:O	2.30	0.64
3:Q:18:GLU:OE1	3:Q:21:ARG:NH1	2.30	0.64
1:X:355:PHE:CE2	1:X:383:LEU:HD11	2.33	0.64
3:S:30:VAL:HG13	3:S:43:ALA:HB2	1.79	0.64
3:Y:28:LYS:NZ	3:Y:46:PRO:CD	2.60	0.64
1:C:374:LEU:HD11	3:I:89:TYR:CD1	2.33	0.64
3:I:18:GLU:HG3	3:I:22:LYS:HE3	1.78	0.64
3:M:99:LEU:O	3:M:102:VAL:HG12	1.97	0.64
2:V:519:GLU:O	2:V:524:ALA:HB3	1.98	0.64
3:W:16:ARG:NH2	3:W:114:GLN:O	2.30	0.64
1:T:348:THR:HB	1:T:351:VAL:HG12	1.80	0.64
2:V:351:VAL:CG1	4:2:861:HOH:O	2.46	0.64
1:Z:301:OZT:H17	1:Z:333:LYS:HZ1	1.62	0.64
3:A:33:LEU:HD23	3:A:33:LEU:H	1.63	0.64
3:M:126:GLU:OE1	3:M:134:LYS:NZ	2.30	0.64
3:Y:161:GLU:O	3:Y:165:ASN:ND2	2.30	0.64
3:Q:11:GLN:HA	3:Q:14:ARG:HD2	1.80	0.63
1:H:382:ARG:NH2	1:H:385:ILE:HD12	2.13	0.63
3:B:159:THR:O	3:B:162:PRO:HD2	1.97	0.63
3:O:92:ARG:HD3	3:O:129:HIS:CE1	2.34	0.63
3:M:112:THR:CG2	3:M:113:GLU:OE1	2.46	0.63
3:W:92:ARG:HB3	3:W:92:ARG:NH1	2.13	0.63
3:Y:18:GLU:OE1	3:Y:21:ARG:NH1	2.32	0.63
1:Z:301:OZT:C7	1:Z:333:LYS:NZ	2.61	0.63
3:D:217:ARG:NH1	3:D:223:ARG:CD	2.50	0.63
3:F:23:GLY:O	3:F:26:ARG:HG2	1.99	0.63
3:K:99:LEU:HA	3:K:102:VAL:HG12	1.81	0.63
3:Q:18:GLU:OE2	3:Q:21:ARG:NH2	2.30	0.63
1:R:301:OZT:C7	1:R:333:LYS:NZ	2.58	0.63
3:M:113:GLU:OE1	3:M:113:GLU:N	2.32	0.63
2:G:379:LYS:NZ	4:G:551:HOH:O	2.30	0.62
1:P:350:ALA:CB	2:V:426:ALA:HB3	2.29	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:350:ALA:CB	1:2:424:ASP:OD2	2.47	0.62
3:S:59:ARG:NH1	3:S:128:ALA:O	2.32	0.62
3:O:140:ARG:NH1	3:O:150:GLU:OE2	2.32	0.62
3:Q:109:THR:HG23	3:Q:113:GLU:OE2	1.99	0.62
3:S:159:THR:HG22	3:S:162:PRO:HG2	1.81	0.62
1:N:359:TYR:HA	1:N:386:MET:CE	2.29	0.62
3:I:19:LEU:CD2	3:S:9:MET:HE3	2.30	0.62
3:O:205:VAL:HG13	3:O:230:LEU:HD23	1.79	0.62
1:J:301:OZT:H37	4:J:772:HOH:O	1.99	0.62
3:I:181:LEU:O	3:I:185:VAL:HG23	1.99	0.62
3:Y:13:MET:HA	3:Y:13:MET:HE3	1.79	0.62
1:N:362:GLU:OE2	1:N:382:ARG:NH1	2.30	0.62
1:L:301:OZT:H17	1:L:333:LYS:HZ1	1.63	0.62
3:Q:48:ARG:HD2	3:Q:48:ARG:H	1.63	0.62
3:Y:179:ASP:O	3:Y:183:ILE:HG13	1.99	0.62
3:Q:48:ARG:CD	3:Q:49:SER:N	2.62	0.62
3:U:116:LYS:NZ	3:U:119:GLU:HG3	2.15	0.62
1:L:382:ARG:HD2	3:M:89:TYR:CE1	2.34	0.62
3:D:217:ARG:HH12	3:D:223:ARG:CD	2.07	0.62
3:O:110:ILE:HG23	3:O:114:GLN:OE1	2.00	0.62
2:V:382:ARG:NH2	4:V:548:HOH:O	2.30	0.61
1:2:382:ARG:HH21	1:2:385:ILE:HD13	1.66	0.61
3:A:121:GLU:HG3	4:A:829:HOH:O	1.98	0.61
1:H:432:GLU:HG2	1:H:437:GLN:HB2	1.81	0.61
1:T:348:THR:O	1:T:351:VAL:HG12	2.01	0.61
3:F:163:ILE:HG23	3:F:187:ALA:O	2.01	0.61
3:B:67:LYS:NZ	3:B:69:ASN:HD21	1.99	0.61
3:O:161:GLU:OE2	3:O:161:GLU:N	2.30	0.61
3:Q:207:SER:O	3:Q:208:LEU:HD23	2.01	0.61
3:W:116:LYS:NZ	3:W:117:PRO:O	2.30	0.61
2:G:479:SER:HB2	2:V:479:SER:HB2	1.81	0.61
1:L:465:ARG:HD3	4:L:676:HOH:O	2.00	0.61
3:Q:116:LYS:CE	3:Q:119:GLU:OE1	2.49	0.61
3:Y:116:LYS:NZ	3:Y:117:PRO:O	2.33	0.61
1:H:366:TYR:CD2	1:H:374:LEU:HD13	2.36	0.60
2:V:465:ARG:HG3	2:V:513:LEU:CD1	2.30	0.60
1:E:301:OZT:H17	1:E:333:LYS:NZ	2.17	0.60
1:E:331:VAL:HG13	1:E:349:ALA:HB2	1.84	0.60
1:J:400:ALA:HB3	4:J:546:HOH:O	2.02	0.60
3:A:161:GLU:HB2	3:A:162:PRO:HD3	1.83	0.60
2:G:301:THR:N	2:G:441:SER:HG	1.99	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:355:PHE:HZ	1:X:383:LEU:HD11	1.66	0.60
3:K:161:GLU:H	3:K:161:GLU:CD	2.04	0.60
1:P:391:LEU:HD12	1:P:391:LEU:O	2.02	0.60
3:F:168:LYS:HB2	3:F:168:LYS:HZ2	1.62	0.60
3:S:229:ALA:O	3:S:233:LEU:CD1	2.50	0.60
3:U:42:VAL:HG13	3:U:188:LEU:HD11	1.83	0.60
2:V:357:ARG:NH2	3:U:87:TYR:O	2.34	0.60
1:C:509:ARG:HG2	4:C:543:HOH:O	2.01	0.60
3:M:59:ARG:NH1	3:M:128:ALA:O	2.35	0.60
1:N:355:PHE:HE2	1:N:383:LEU:CD1	2.15	0.59
3:D:112:THR:HG23	3:Q:115:ALA:HB3	1.82	0.59
3:O:129:HIS:HE1	4:O:746:HOH:O	1.85	0.59
3:Q:179:ASP:O	3:Q:183:ILE:CD1	2.50	0.59
1:N:301:OZT:H17	1:N:333:LYS:HZ3	1.65	0.59
1:T:331:VAL:HG13	1:T:349:ALA:HB1	1.85	0.59
3:F:18:GLU:OE1	3:F:22:LYS:HG3	2.02	0.59
3:U:18:GLU:OE2	3:U:21:ARG:NH1	2.35	0.59
3:W:205:VAL:HG22	3:W:208:LEU:HG	1.85	0.59
1:H:382:ARG:HD2	3:B:89:TYR:CE1	2.37	0.59
2:G:477:ASP:OD1	2:V:329:ARG:NH2	2.36	0.59
3:K:161:GLU:OE1	3:K:161:GLU:N	2.30	0.59
3:S:116:LYS:NZ	3:S:119:GLU:OE1	2.30	0.59
3:1:230:LEU:C	3:1:234:LEU:HD11	2.23	0.59
3:K:47:SER:OG	3:M:149:ASP:HB3	2.03	0.59
1:H:465:ARG:HG3	1:H:513:LEU:HD22	1.83	0.59
3:D:114:GLN:NE2	3:D:114:GLN:CA	2.64	0.59
3:O:152:HIS:NE2	3:O:173:GLU:OE1	2.36	0.59
1:P:346:ALA:HA	4:P:553:HOH:O	2.02	0.59
1:Z:444:LEU:HB2	4:Z:549:HOH:O	2.03	0.59
3:O:177:LEU:HG	3:O:233:LEU:HD21	1.85	0.59
2:V:382:ARG:NH2	2:V:385:ILE:CD1	2.66	0.58
2:V:456:GLN:CD	2:V:465:ARG:NH2	2.56	0.58
3:S:112:THR:HG22	3:S:113:GLU:CG	2.26	0.58
3:Y:173:GLU:HG2	3:Y:174:ASN:ND2	2.19	0.58
1:R:357:ARG:O	1:R:361:VAL:HG23	2.02	0.58
1:R:429:TRP:HD1	4:R:614:HOH:O	1.86	0.58
3:F:21:ARG:NH1	3:F:21:ARG:CG	2.50	0.58
1:N:424:ASP:OD1	1:N:428:GLY:N	2.36	0.58
3:A:159:THR:O	3:A:162:PRO:HD2	2.03	0.58
3:I:189:ARG:HD3	3:I:189:ARG:C	2.23	0.58
3:Q:181:LEU:HD12	3:Q:182:ARG:N	2.16	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:W:172:ALA:HB3	3:W:175:ALA:HB2	1.84	0.58
3:F:72:ASP:O	3:F:76:ARG:HG3	2.04	0.58
3:Q:48:ARG:HD2	3:Q:49:SER:N	2.16	0.58
3:S:229:ALA:O	3:S:233:LEU:HD13	2.04	0.58
3:1:163:ILE:HG23	3:1:187:ALA:HB1	1.85	0.58
3:U:116:LYS:HZ1	3:U:119:GLU:HG3	1.69	0.58
3:I:16:ARG:NH2	3:I:114:GLN:O	2.36	0.58
1:R:388:ARG:C	1:R:390:ASN:H	2.07	0.58
3:A:149:ASP:CG	3:O:48:ARG:NH1	2.57	0.58
3:I:19:LEU:CD2	3:S:9:MET:CE	2.81	0.58
3:Q:45:ASN:ND2	3:Q:52:LYS:HG3	2.18	0.57
1:H:382:ARG:NH2	1:H:385:ILE:CD1	2.65	0.57
3:D:121:GLU:OE2	3:D:156:MET:HG2	2.03	0.57
3:Q:25:ALA:O	3:Q:158:GLY:HA2	2.04	0.57
1:J:301:OZT:H17	1:J:333:LYS:HZ1	1.68	0.57
1:X:345:ILE:HD11	1:X:355:PHE:CD2	2.38	0.57
1:X:366:TYR:CD2	1:X:374:LEU:HD13	2.39	0.57
1:E:464:LEU:O	1:E:468:VAL:HG23	2.04	0.57
1:T:350:ALA:O	1:T:353:VAL:HG12	2.03	0.57
3:O:163:ILE:HG23	3:O:187:ALA:O	2.05	0.57
3:S:170:SER:OG	3:S:183:ILE:HG23	2.05	0.57
3:B:18:GLU:HG2	3:B:22:LYS:HE3	1.85	0.57
3:O:182:ARG:HH21	3:O:235:VAL:HA	1.70	0.57
3:U:163:ILE:CD1	3:U:191:GLY:HA3	2.32	0.57
3:W:176:SER:HB3	3:W:179:ASP:OD1	2.04	0.57
3:Y:11:GLN:O	3:Y:14:ARG:HB3	2.04	0.57
1:C:465:ARG:HG3	1:C:513:LEU:HD22	1.86	0.57
1:X:301:OZT:C7	1:X:333:LYS:HZ1	2.10	0.57
3:Q:172:ALA:CB	3:Q:175:ALA:HB2	2.34	0.57
1:N:359:TYR:HD1	1:N:386:MET:HE3	1.70	0.57
1:N:355:PHE:CE2	1:N:383:LEU:HD11	2.35	0.56
1:N:383:LEU:O	1:N:387:VAL:HG23	2.04	0.56
3:S:205:VAL:C	3:S:207:SER:H	2.09	0.56
1:E:348:THR:HB	1:E:351:VAL:HG23	1.87	0.56
1:J:355:PHE:CD2	1:J:386:MET:HE1	2.41	0.56
1:P:301:OZT:H17	1:P:333:LYS:NZ	2.20	0.56
1:T:331:VAL:HG11	1:T:349:ALA:CB	2.35	0.56
3:Q:159:THR:O	3:Q:163:ILE:CD1	2.53	0.56
1:Z:366:TYR:CE2	1:Z:374:LEU:HD13	2.40	0.56
3:Y:173:GLU:CG	3:Y:174:ASN:ND2	2.69	0.56
3:K:99:LEU:O	3:K:102:VAL:CG1	2.53	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:62:PHE:C	3:M:62:PHE:CD2	2.78	0.56
3:O:159:THR:HG22	3:O:162:PRO:CG	2.34	0.56
3:S:92:ARG:HH11	3:S:92:ARG:HB3	1.69	0.56
3:A:137:GLU:OE2	3:O:48:ARG:NH2	2.30	0.56
3:K:30:VAL:HG13	3:K:43:ALA:HB2	1.86	0.56
3:M:67:LYS:HG2	3:M:69:ASN:ND2	2.20	0.56
2:G:382:ARG:HD2	3:W:89:TYR:CE1	2.41	0.56
1:2:426:ALA:CB	4:2:861:HOH:O	2.53	0.56
1:C:354:GLU:OE2	1:C:355:PHE:CA	2.53	0.56
1:R:388:ARG:O	1:R:390:ASN:N	2.40	0.56
3:F:44:GLU:CG	3:F:188:LEU:HD22	2.36	0.56
3:I:52:LYS:NZ	4:I:303:HOH:O	2.30	0.56
1:C:452:LYS:HG3	1:R:452:LYS:HB2	1.87	0.55
3:D:217:ARG:HH12	3:D:223:ARG:CB	2.14	0.55
3:A:137:GLU:HG2	3:O:48:ARG:CZ	2.35	0.55
3:Q:116:LYS:HE3	3:Q:119:GLU:OE1	2.05	0.55
3:S:181:LEU:HD23	3:S:233:LEU:HB3	1.88	0.55
2:V:350:ALA:HB2	1:2:424:ASP:OD2	2.06	0.55
2:V:382:ARG:HH21	2:V:385:ILE:HD12	1.70	0.55
3:B:159:THR:HG22	3:B:162:PRO:CD	2.36	0.55
3:F:24:ILE:O	3:F:24:ILE:HG22	2.06	0.55
3:W:97:ARG:O	3:W:101:ASN:HB2	2.07	0.55
1:E:449:SER:OG	1:E:473:ASP:OD2	2.20	0.55
2:V:362:GLU:OE2	2:V:382:ARG:CD	2.51	0.55
3:D:109:THR:O	3:D:113:GLU:N	2.36	0.55
1:C:392:ALA:HB3	4:C:578:HOH:O	2.06	0.55
3:B:115:ALA:HB3	3:I:112:THR:CG2	2.37	0.55
3:I:48:ARG:HD2	4:I:977:HOH:O	2.05	0.55
3:1:30:VAL:HG13	3:1:43:ALA:HB2	1.88	0.55
1:H:390:ASN:ND2	1:H:393:ALA:CB	2.69	0.55
3:U:14:ARG:O	3:U:18:GLU:HB2	2.05	0.55
3:K:99:LEU:O	3:K:102:VAL:HG12	2.07	0.55
3:O:24:ILE:HG22	3:O:157:GLY:HA2	1.88	0.55
3:F:16:ARG:CA	3:F:16:ARG:CZ	2.85	0.55
3:S:161:GLU:HB2	3:S:162:PRO:HD3	1.89	0.55
1:C:354:GLU:OE2	1:C:355:PHE:N	2.39	0.55
3:U:31:VAL:CG2	3:U:188:LEU:HD21	2.35	0.55
3:U:181:LEU:O	3:U:185:VAL:HG23	2.06	0.55
3:W:205:VAL:CG2	3:W:207:SER:H	1.94	0.55
3:1:225:ILE:CG2	3:1:233:LEU:HD12	2.36	0.55
1:N:401:LEU:HD22	1:N:423:PHE:O	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:159:THR:HG22	3:F:162:PRO:CG	2.37	0.55
3:M:37:GLY:HA3	4:M:249:HOH:O	2.07	0.54
3:O:46:PRO:HD2	3:O:47:SER:H	1.72	0.54
1:J:428:GLY:HA2	1:T:350:ALA:HB1	1.88	0.54
1:C:477:ASP:OD1	1:E:329:ARG:NH2	2.38	0.54
1:T:382:ARG:HH21	1:T:385:ILE:HD13	1.73	0.54
3:I:18:GLU:OE1	3:I:18:GLU:HA	2.08	0.54
3:K:159:THR:HG22	3:K:162:PRO:CD	2.37	0.54
3:Q:116:LYS:NZ	3:Q:119:GLU:OE1	2.39	0.54
1:J:373:PRO:HD3	4:J:551:HOH:O	2.08	0.54
3:A:59:ARG:NH2	3:A:217:ARG:O	2.31	0.54
3:F:16:ARG:CZ	3:F:16:ARG:HA	2.38	0.54
3:K:106:THR:O	3:K:110:ILE:HG13	2.07	0.54
1:L:390:ASN:ND2	1:L:393:ALA:HB3	2.22	0.54
3:F:159:THR:CG2	3:F:162:PRO:HG2	2.38	0.54
1:H:370:GLU:O	3:B:97:ARG:NH1	2.40	0.54
3:O:112:THR:CG2	3:U:115:ALA:CB	2.82	0.54
3:S:161:GLU:CD	3:S:161:GLU:N	2.60	0.54
2:V:320:SER:HB2	2:V:331:VAL:HG21	1.90	0.54
3:F:14:ARG:HH11	3:F:14:ARG:HB2	1.73	0.54
3:Y:52:LYS:NZ	4:Y:415:HOH:O	2.30	0.54
1:E:432:GLU:OE2	1:E:437:GLN:NE2	2.40	0.53
1:N:376:PHE:O	1:N:380:ILE:HG13	2.08	0.53
3:A:205:VAL:HG13	3:A:234:LEU:HD23	1.90	0.53
3:F:159:THR:HG22	3:F:162:PRO:HG2	1.89	0.53
3:K:116:LYS:HE3	3:M:111:PHE:HE2	1.73	0.53
3:K:161:GLU:CD	3:K:161:GLU:N	2.62	0.53
3:O:41:PHE:HB3	3:O:53:ILE:HD13	1.89	0.53
3:U:206:ALA:O	3:U:207:SER:HB3	2.08	0.53
1:H:388:ARG:HD2	1:H:426:ALA:O	2.08	0.53
1:L:390:ASN:CG	1:L:390:ASN:O	2.46	0.53
1:T:320:SER:HB2	1:T:331:VAL:HG21	1.91	0.53
2:V:374:LEU:HD11	3:O:89:TYR:CD1	2.44	0.53
1:2:399:LEU:HB2	4:2:668:HOH:O	2.07	0.53
3:S:159:THR:O	3:S:163:ILE:HG13	2.07	0.53
3:A:205:VAL:HG13	3:A:234:LEU:CD2	2.39	0.53
3:K:116:LYS:HG2	3:K:117:PRO:N	2.23	0.53
3:S:90:ASP:CB	3:S:93:ASP:OD2	2.57	0.53
1:P:320:SER:HB2	1:P:331:VAL:HG21	1.90	0.53
1:2:432:GLU:HB3	4:2:580:HOH:O	2.08	0.53
3:Q:163:ILE:HG23	3:Q:187:ALA:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:121:GLU:HG2	3:D:156:MET:SD	2.49	0.53
1:L:432:GLU:HG3	1:L:437:GLN:HB2	1.90	0.53
1:R:362:GLU:OE2	1:R:382:ARG:NH1	2.41	0.53
3:F:16:ARG:CB	3:F:16:ARG:CZ	2.84	0.53
3:K:92:ARG:HH21	3:K:129:HIS:CD2	2.24	0.53
3:Q:14:ARG:HG3	4:Q:982:HOH:O	2.09	0.53
3:Q:11:GLN:O	3:Q:11:GLN:HG3	2.08	0.53
3:U:230:LEU:HD12	4:U:747:HOH:O	2.08	0.53
3:Y:59:ARG:NH1	3:Y:128:ALA:O	2.35	0.53
2:V:435:GLY:N	4:V:553:HOH:O	2.30	0.53
3:D:112:THR:HG22	3:Q:115:ALA:HB3	1.90	0.53
3:M:56:LEU:HD11	3:M:62:PHE:HB2	1.89	0.53
3:Q:205:VAL:CG1	3:Q:206:ALA:N	2.37	0.53
3:U:206:ALA:O	3:U:207:SER:CB	2.56	0.53
3:F:44:GLU:HG3	3:F:188:LEU:HD22	1.91	0.53
3:O:45:ASN:OD1	3:O:46:PRO:HD2	2.08	0.53
3:U:67:LYS:HD2	4:U:898:HOH:O	2.09	0.53
1:C:319:ARG:NH1	1:C:479:SER:O	2.43	0.52
3:F:26:ARG:CZ	3:F:192:SER:HA	2.38	0.52
3:O:133:THR:HG22	4:O:961:HOH:O	2.08	0.52
3:Y:28:LYS:NZ	3:Y:46:PRO:HD2	2.22	0.52
2:V:348:THR:CB	2:V:351:VAL:CG2	2.86	0.52
3:U:20:ALA:O	3:U:24:ILE:HG13	2.09	0.52
2:G:345:ILE:N	2:G:345:ILE:CD1	2.71	0.52
3:F:161:GLU:HB2	3:F:162:PRO:HD3	1.92	0.52
3:K:99:LEU:HA	3:K:102:VAL:CG1	2.39	0.52
3:M:173:GLU:OE1	3:M:173:GLU:HA	2.09	0.52
3:O:181:LEU:HD22	3:O:233:LEU:HD23	1.90	0.52
3:Q:180:ALA:CA	3:Q:183:ILE:HD12	2.16	0.52
1:R:348:THR:HG21	1:Z:424:ASP:OD2	2.10	0.52
1:Z:301:OZT:O	1:Z:440:GLY:HA3	2.10	0.52
3:B:170:SER:OG	3:B:183:ILE:HG23	2.09	0.52
3:I:223:ARG:HG2	4:I:769:HOH:O	2.10	0.52
3:U:116:LYS:NZ	3:U:119:GLU:OE1	2.42	0.52
3:F:51:GLN:CG	3:F:209:GLU:OE2	2.49	0.52
3:U:163:ILE:HG12	3:U:191:GLY:CA	2.33	0.52
3:U:205:VAL:CG1	3:U:206:ALA:N	2.71	0.52
1:N:301:OZT:H17	1:N:333:LYS:HZ1	1.75	0.52
3:I:142:THR:HG22	3:I:146:SER:HB2	1.92	0.52
3:M:95:THR:HG21	4:M:700:HOH:O	2.10	0.52
3:O:51:GLN:HB3	3:O:209:GLU:OE2	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:U:46:PRO:HA	3:U:207:SER:HA	1.92	0.52
2:G:429:TRP:O	1:X:350:ALA:HB2	2.09	0.52
1:2:382:ARG:HH21	1:2:385:ILE:CD1	2.23	0.52
3:A:33:LEU:N	3:A:33:LEU:CD2	2.73	0.52
3:W:30:VAL:HG13	3:W:43:ALA:HB2	1.92	0.52
3:W:99:LEU:HA	3:W:102:VAL:HG12	1.92	0.52
3:Y:59:ARG:HD2	3:Y:129:HIS:HA	1.92	0.51
1:Z:465:ARG:HG3	1:Z:513:LEU:HD22	1.91	0.51
3:B:205:VAL:HG22	3:B:230:LEU:HG	1.91	0.51
3:M:45:ASN:C	3:M:45:ASN:OD1	2.47	0.51
1:H:301:OZT:H17	1:H:333:LYS:HZ1	1.71	0.51
1:R:424:ASP:OD1	1:R:428:GLY:N	2.32	0.51
2:V:382:ARG:NH2	2:V:385:ILE:HD13	2.24	0.51
3:A:141:ILE:HD12	3:A:141:ILE:N	2.25	0.51
3:A:52:LYS:NZ	4:A:651:HOH:O	2.31	0.51
3:B:205:VAL:HG23	3:B:234:LEU:CD1	2.40	0.51
3:M:173:GLU:HB3	3:M:174:ASN:HD22	1.75	0.51
3:O:112:THR:HG22	3:U:115:ALA:CB	2.38	0.51
3:D:117:PRO:HG3	4:D:930:HOH:O	2.05	0.51
3:F:99:LEU:O	3:F:102:VAL:HG12	2.11	0.51
3:M:41:PHE:CB	3:M:53:ILE:HD13	2.38	0.51
1:T:331:VAL:HG11	1:T:349:ALA:HB1	1.93	0.51
3:O:159:THR:O	3:O:162:PRO:HD2	2.11	0.51
1:C:351:VAL:O	1:C:355:PHE:HB2	2.11	0.51
2:G:347:GLY:O	2:G:348:THR:C	2.47	0.51
1:L:441:SER:OG	1:L:478:ASP:OD2	2.21	0.51
3:Y:51:GLN:CG	3:Y:209:GLU:OE2	2.58	0.51
3:1:163:ILE:HG12	3:1:187:ALA:O	2.11	0.51
1:J:382:ARG:HH21	1:J:385:ILE:HD13	1.76	0.51
1:N:357:ARG:O	1:N:361:VAL:HG23	2.10	0.51
2:V:337:THR:HG21	2:V:343:THR:OG1	2.11	0.51
3:A:167:LEU:O	3:A:171:TYR:N	2.39	0.51
3:U:45:ASN:ND2	3:U:209:GLU:OE1	2.27	0.51
1:N:400:ALA:O	1:N:402:PRO:HD3	2.11	0.51
1:T:301:OZT:C7	1:T:333:LYS:HZ1	2.17	0.51
1:X:434:GLU:HB2	4:X:544:HOH:O	2.11	0.51
3:A:166:ALA:O	3:A:170:SER:HB2	2.11	0.51
3:F:21:ARG:C	3:F:21:ARG:CD	2.68	0.51
3:F:189:ARG:O	3:F:192:SER:HB3	2.11	0.51
3:K:133:THR:HA	4:K:803:HOH:O	2.10	0.51
3:1:225:ILE:HA	4:1:604:HOH:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:432:GLU:HG3	1:C:437:GLN:HB2	1.92	0.50
4:O:853:HOH:O	3:U:67:LYS:HE2	2.12	0.50
2:G:382:ARG:HH21	2:G:385:ILE:HD13	1.75	0.50
1:P:366:TYR:CE2	1:P:374:LEU:HD13	2.46	0.50
3:A:30:VAL:HG13	3:A:43:ALA:HB2	1.94	0.50
3:M:106:THR:O	3:M:110:ILE:HG13	2.11	0.50
3:U:150:GLU:OE1	3:U:154:VAL:HG22	2.11	0.50
3:F:28:LYS:HB3	3:F:44:GLU:HB2	1.91	0.50
3:Y:99:LEU:O	3:Y:102:VAL:HG12	2.12	0.50
3:Y:106:THR:O	3:Y:110:ILE:HG13	2.11	0.50
1:C:319:ARG:CG	1:C:320:SER:N	2.73	0.50
2:G:350:ALA:C	2:G:352:ALA:N	2.65	0.50
2:V:350:ALA:HB3	1:2:424:ASP:OD2	2.10	0.50
3:U:59:ARG:HD2	3:U:129:HIS:HA	1.94	0.50
3:W:14:ARG:HG3	3:W:16:ARG:H	1.74	0.50
2:V:516:ALA:O	2:V:520:SER:OG	2.30	0.50
3:K:90:ASP:HB3	3:K:93:ASP:OD2	2.12	0.50
3:S:161:GLU:N	3:S:161:GLU:OE2	2.30	0.50
1:X:366:TYR:CZ	1:X:374:LEU:HD13	2.46	0.50
3:A:59:ARG:HD2	3:A:129:HIS:HA	1.93	0.50
3:B:30:VAL:HG13	3:B:43:ALA:HB2	1.94	0.50
1:R:354:GLU:OE2	1:R:354:GLU:HA	2.12	0.50
1:T:348:THR:O	1:T:351:VAL:CG1	2.60	0.50
3:I:99:LEU:O	3:I:102:VAL:HG12	2.12	0.50
3:I:115:ALA:O	3:S:9:MET:SD	2.69	0.50
3:1:110:ILE:HG12	3:1:114:GLN:NE2	2.27	0.50
1:C:357:ARG:O	1:C:361:VAL:HG23	2.12	0.49
1:N:422:SER:OG	1:N:432:GLU:OE2	2.30	0.49
3:M:67:LYS:HG2	3:M:69:ASN:HD21	1.77	0.49
3:Y:133:THR:O	3:Y:133:THR:CG2	2.55	0.49
1:E:382:ARG:HD2	3:K:89:TYR:CE1	2.48	0.49
1:R:325:MET:CE	1:Z:444:LEU:HD21	2.41	0.49
1:T:479:SER:HB2	1:Z:479:SER:HB2	1.94	0.49
1:2:317:ASP:OD2	1:2:333:LYS:NZ	2.45	0.49
3:O:159:THR:CG2	3:O:162:PRO:HG2	2.43	0.49
1:C:301:OZT:C7	1:C:333:LYS:HZ1	2.22	0.49
2:G:366:TYR:CD2	2:G:374:LEU:HD13	2.47	0.49
3:A:45:ASN:O	3:A:207:SER:O	2.29	0.49
3:W:17:SER:OG	3:W:143:TYR:OH	2.27	0.49
3:Q:181:LEU:O	3:Q:185:VAL:HG23	2.12	0.49
2:G:350:ALA:O	2:G:352:ALA:N	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Y:31:VAL:HG23	3:Y:188:LEU:HD21	1.94	0.49
1:L:354:GLU:OE1	1:L:354:GLU:HA	2.13	0.49
1:L:424:ASP:HB2	4:L:729:HOH:O	2.12	0.49
1:N:432:GLU:CD	1:N:437:GLN:HE21	2.15	0.49
2:V:456:GLN:NE2	2:V:465:ARG:HH22	2.10	0.49
1:E:331:VAL:HG13	1:E:349:ALA:CB	2.42	0.49
2:V:425:ALA:HB3	4:V:964:HOH:O	2.11	0.49
3:A:27:ALA:HB1	4:A:651:HOH:O	2.12	0.49
3:W:59:ARG:NH2	3:W:217:ARG:O	2.38	0.49
2:G:348:THR:O	2:G:351:VAL:HG13	2.12	0.49
1:T:483:GLY:HA2	4:T:60:HOH:O	2.12	0.49
3:D:149:ASP:OD2	3:Q:48:ARG:CZ	2.61	0.49
3:Y:10:GLU:HA	3:Y:13:MET:HB2	1.95	0.49
3:Y:121:GLU:HG3	4:Y:368:HOH:O	2.11	0.49
2:G:487:VAL:CG1	2:V:521:ARG:HB3	2.40	0.49
1:R:465:ARG:HD2	4:R:950:HOH:O	2.13	0.49
1:2:392:ALA:HB3	4:2:542:HOH:O	2.13	0.49
3:F:47:SER:HB2	3:W:149:ASP:OD2	2.13	0.49
3:F:152:HIS:HB3	3:F:171:TYR:CZ	2.48	0.49
1:C:448:SER:HB3	1:R:448:SER:HB3	1.94	0.49
2:V:351:VAL:HG12	4:2:861:HOH:O	2.10	0.49
1:2:465:ARG:HG3	1:2:513:LEU:HD22	1.94	0.49
3:M:90:ASP:O	3:M:93:ASP:HB2	2.12	0.48
3:U:162:PRO:HB2	3:U:191:GLY:CA	2.38	0.48
3:D:58:ASP:OD1	3:D:91:ARG:NH2	2.46	0.48
3:K:159:THR:O	3:K:163:ILE:HG13	2.12	0.48
3:Y:28:LYS:HZ3	3:Y:46:PRO:CD	2.26	0.48
1:C:374:LEU:HD11	3:I:89:TYR:HD1	1.78	0.48
1:L:351:VAL:HG21	4:L:545:HOH:O	2.14	0.48
1:N:515:ARG:HD3	4:N:541:HOH:O	2.12	0.48
1:T:348:THR:HB	1:T:351:VAL:CG1	2.42	0.48
3:I:144:ASP:OD2	3:I:146:SER:OG	2.32	0.48
3:M:205:VAL:HG12	3:M:207:SER:H	1.77	0.48
1:E:348:THR:CB	1:E:351:VAL:HG23	2.44	0.48
3:F:163:ILE:HD13	3:F:188:LEU:HA	1.94	0.48
3:M:30:VAL:HG13	3:M:43:ALA:HB2	1.95	0.48
3:W:142:THR:OG1	3:W:146:SER:HB2	2.13	0.48
1:E:335:TYR:OH	1:E:353:VAL:HG22	2.14	0.48
3:K:59:ARG:HD2	3:K:129:HIS:HA	1.94	0.48
3:M:174:ASN:HD22	3:M:174:ASN:N	2.10	0.48
2:G:350:ALA:O	2:G:351:VAL:C	2.50	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:382:ARG:HH21	2:G:385:ILE:CD1	2.26	0.48
1:P:382:ARG:HH21	1:P:385:ILE:HD13	1.76	0.48
3:B:67:LYS:HZ3	3:B:69:ASN:HD21	1.61	0.48
3:F:125:ALA:HB2	3:F:138:LEU:HD23	1.95	0.48
3:I:55:GLU:HB2	3:I:222:PHE:CG	2.47	0.48
3:K:155:VAL:HG12	3:K:160:THR:HG22	1.96	0.48
1:H:366:TYR:CE2	1:H:374:LEU:HD13	2.49	0.48
3:I:69:ASN:H	3:I:69:ASN:HD22	1.61	0.48
3:M:59:ARG:HH12	3:M:215:ALA:HA	1.77	0.48
3:S:181:LEU:HD23	3:S:233:LEU:CB	2.44	0.48
1:H:301:OZT:H17	1:H:333:LYS:CE	2.44	0.48
1:L:301:OZT:C7	1:L:333:LYS:NZ	2.71	0.48
1:X:318:ARG:HD3	1:X:493:THR:HG23	1.95	0.48
3:I:203:LEU:N	3:I:203:LEU:HD12	2.29	0.48
3:K:73:ASN:ND2	3:M:105:GLN:NE2	2.61	0.48
3:K:229:ALA:O	3:K:233:LEU:HD13	2.13	0.48
2:V:513:LEU:HD13	2:V:513:LEU:HA	1.68	0.48
3:B:19:LEU:HD13	3:I:10:GLU:HG2	1.95	0.48
3:I:42:VAL:HG13	3:I:210:VAL:HG22	1.96	0.48
3:K:207:SER:O	3:K:207:SER:OG	2.32	0.48
1:C:437:GLN:OE1	1:C:447:LYS:HD2	2.14	0.48
3:Q:10:GLU:HG3	3:Y:15:GLU:CG	2.44	0.48
3:U:163:ILE:HG12	3:U:191:GLY:N	2.28	0.48
3:Y:12:ALA:C	3:Y:14:ARG:N	2.67	0.48
3:K:159:THR:HG22	3:K:162:PRO:HD2	1.94	0.47
3:M:217:ARG:HD2	3:M:223:ARG:HD3	1.96	0.47
3:U:31:VAL:HG23	3:U:188:LEU:CD2	2.43	0.47
3:Y:45:ASN:C	3:Y:45:ASN:OD1	2.51	0.47
2:G:354:GLU:OE2	1:N:429:TRP:NE1	2.46	0.47
1:Z:353:VAL:O	1:Z:357:ARG:HB2	2.14	0.47
3:K:176:SER:HB3	3:K:179:ASP:OD2	2.15	0.47
3:U:116:LYS:HE2	3:U:119:GLU:OE1	2.15	0.47
2:G:362:GLU:HG3	4:G:547:HOH:O	2.14	0.47
1:N:362:GLU:OE2	1:N:382:ARG:HD3	2.14	0.47
1:T:357:ARG:NH2	3:S:87:TYR:O	2.45	0.47
3:S:181:LEU:O	3:S:185:VAL:HG23	2.15	0.47
3:1:234:LEU:CD1	3:1:234:LEU:H	2.09	0.47
1:P:350:ALA:CB	2:V:426:ALA:CB	2.91	0.47
3:F:59:ARG:HD2	3:F:129:HIS:HA	1.97	0.47
3:S:116:LYS:HG2	3:S:117:PRO:HD2	1.95	0.47
3:S:182:ARG:HH21	3:S:235:VAL:C	2.18	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Y:109:THR:O	3:Y:113:GLU:HB2	2.13	0.47
2:G:464:LEU:HD21	2:G:505:VAL:HG11	1.96	0.47
1:R:366:TYR:CZ	1:R:374:LEU:HD13	2.50	0.47
1:T:366:TYR:CE2	1:T:374:LEU:HD13	2.49	0.47
2:V:301:THR:O	2:V:440:GLY:HA3	2.14	0.47
2:V:382:ARG:NH2	2:V:385:ILE:HD12	2.27	0.47
1:X:319:ARG:CG	1:X:320:SER:N	2.77	0.47
3:F:16:ARG:NH2	3:F:19:LEU:HB2	2.30	0.47
1:C:448:SER:CB	1:R:448:SER:HB3	2.44	0.47
2:V:366:TYR:CD2	2:V:374:LEU:HD13	2.50	0.47
3:B:59:ARG:HD2	3:B:129:HIS:HA	1.96	0.47
3:F:67:LYS:HE2	3:W:146:SER:OG	2.13	0.47
3:I:73:ASN:HD21	3:S:105:GLN:HG3	1.79	0.47
3:O:10:GLU:HG3	3:U:15:GLU:HG3	1.97	0.47
3:O:181:LEU:O	3:O:185:VAL:HG23	2.15	0.47
3:W:205:VAL:HG23	3:W:206:ALA:N	2.29	0.47
3:Y:163:ILE:HG23	3:Y:187:ALA:C	2.34	0.47
1:L:331:VAL:HG13	1:L:349:ALA:HA	1.97	0.47
3:A:35:TYR:CE1	3:A:37:GLY:CA	2.97	0.47
3:F:94:VAL:HA	3:F:98:GLN:NE2	2.29	0.47
3:O:159:THR:HG22	3:O:162:PRO:HG2	1.97	0.47
2:V:348:THR:HG22	2:V:351:VAL:CG1	2.45	0.47
3:S:210:VAL:HG12	3:S:211:ALA:N	2.29	0.47
1:L:355:PHE:HE2	1:L:383:LEU:HD11	1.79	0.47
1:T:382:ARG:HH21	1:T:385:ILE:CD1	2.27	0.47
1:2:350:ALA:HA	1:2:353:VAL:HG12	1.96	0.47
1:C:320:SER:HB2	1:C:331:VAL:HG21	1.96	0.46
1:P:364:GLU:HB2	4:P:629:HOH:O	2.14	0.46
1:P:432:GLU:HG3	1:P:437:GLN:HB2	1.97	0.46
3:S:17:SER:OG	3:S:21:ARG:NH1	2.47	0.46
1:E:301:OZT:H17	1:E:333:LYS:HZ1	1.79	0.46
1:E:507:GLU:HG2	4:E:846:HOH:O	2.16	0.46
3:K:99:LEU:CA	3:K:102:VAL:HG12	2.44	0.46
3:O:170:SER:HB2	3:O:183:ILE:HG23	1.95	0.46
1:X:355:PHE:HZ	1:X:383:LEU:CD1	2.24	0.46
3:B:36:ALA:HA	3:B:174:ASN:OD1	2.15	0.46
3:Y:56:LEU:HG	3:Y:62:PHE:HB2	1.98	0.46
3:Y:129:HIS:O	3:Y:132:GLU:HB2	2.15	0.46
1:N:437:GLN:HG3	1:N:438:ALA:N	2.30	0.46
1:P:350:ALA:HB2	2:V:426:ALA:HB3	1.97	0.46
2:V:347:GLY:O	2:V:348:THR:C	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:494:ALA:HB3	1:X:510:ILE:HD11	1.97	0.46
3:F:102:VAL:CG1	3:F:103:TYR:N	2.77	0.46
3:M:67:LYS:CE	3:M:69:ASN:HD21	2.25	0.46
3:M:174:ASN:N	3:M:174:ASN:ND2	2.63	0.46
3:D:69:ASN:H	3:D:69:ASN:HD22	1.63	0.46
3:D:90:ASP:O	3:D:93:ASP:HB3	2.15	0.46
3:K:47:SER:OG	3:M:149:ASP:OD2	2.33	0.46
3:Q:13:MET:CE	3:Q:111:PHE:HE2	2.29	0.46
1:E:309:PRO:HG2	1:E:458:THR:O	2.16	0.46
2:V:465:ARG:HG2	2:V:465:ARG:O	2.15	0.46
3:M:110:ILE:O	3:M:114:GLN:HB2	2.15	0.46
3:W:56:LEU:HG	3:W:62:PHE:HB2	1.97	0.46
1:H:301:OZT:H27	1:H:333:LYS:HE2	1.97	0.46
1:H:362:GLU:HG3	4:H:546:HOH:O	2.15	0.46
1:R:388:ARG:C	1:R:390:ASN:N	2.68	0.46
3:K:47:SER:OG	3:M:149:ASP:HB2	2.13	0.46
1:L:448:SER:CB	1:P:448:SER:HB3	2.45	0.46
1:X:301:OZT:H27	1:X:333:LYS:NZ	2.29	0.46
3:O:69:ASN:HD22	3:O:69:ASN:H	1.64	0.46
1:H:362:GLU:OE2	1:H:382:ARG:HD3	2.16	0.46
1:R:362:GLU:OE2	1:R:382:ARG:HD3	2.16	0.46
1:Z:382:ARG:HH21	1:Z:385:ILE:HD13	1.81	0.46
3:F:14:ARG:HB2	3:F:14:ARG:NH1	2.31	0.46
3:O:46:PRO:CD	3:O:47:SER:H	2.29	0.46
1:T:464:LEU:HD21	1:T:505:VAL:HG11	1.98	0.46
2:V:350:ALA:HB1	1:2:428:GLY:HA3	1.98	0.46
1:2:426:ALA:HB1	4:2:861:HOH:O	2.16	0.46
3:D:116:LYS:NZ	3:D:119:GLU:OE1	2.43	0.46
3:I:59:ARG:HD2	3:I:128:ALA:O	2.16	0.46
3:Q:48:ARG:CG	3:Q:49:SER:N	2.79	0.46
3:U:110:ILE:HG21	3:U:118:TYR:CD1	2.51	0.46
1:N:361:VAL:O	1:N:365:HIS:HB2	2.16	0.45
1:P:307:LYS:HE2	4:P:214:HOH:O	2.16	0.45
1:R:423:PHE:HA	1:R:428:GLY:O	2.16	0.45
3:A:15:GLU:HB3	4:A:1024:HOH:O	2.15	0.45
3:B:115:ALA:HB3	3:I:112:THR:HG22	1.97	0.45
1:E:335:TYR:CZ	1:E:353:VAL:HG22	2.51	0.45
1:L:382:ARG:HH22	1:L:385:ILE:HD13	1.74	0.45
3:D:111:PHE:CE2	3:D:144:ASP:HB2	2.51	0.45
3:F:59:ARG:NH2	3:F:217:ARG:O	2.39	0.45
3:F:74:LEU:HD21	3:F:107:LEU:HD11	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:161:GLU:HB2	3:K:162:PRO:HD3	1.98	0.45
3:Q:40:LEU:HD21	3:Q:181:LEU:HA	1.97	0.45
3:S:205:VAL:C	3:S:207:SER:N	2.69	0.45
3:U:21:ARG:HG3	3:U:22:LYS:N	2.30	0.45
3:W:67:LYS:NZ	3:W:69:ASN:HD21	2.14	0.45
1:E:320:SER:HB2	1:E:331:VAL:HG21	1.97	0.45
1:E:382:ARG:HH21	1:E:385:ILE:HD13	1.81	0.45
1:E:432:GLU:HB3	4:E:545:HOH:O	2.16	0.45
1:N:307:LYS:CD	4:N:542:HOH:O	2.62	0.45
1:P:383:LEU:O	1:P:387:VAL:HG23	2.16	0.45
3:D:130:TYR:CE1	3:D:216:ASN:O	2.70	0.45
4:B:737:HOH:O	3:I:9:MET:HE3	2.15	0.45
3:K:45:ASN:OD1	3:K:46:PRO:HD2	2.17	0.45
1:C:329:ARG:O	1:C:490:ILE:HG21	2.16	0.45
1:P:350:ALA:HB3	2:V:426:ALA:CB	2.46	0.45
1:Z:465:ARG:HD2	4:Z:576:HOH:O	2.16	0.45
3:A:45:ASN:N	3:A:207:SER:O	2.41	0.45
1:R:353:VAL:CG2	4:R:548:HOH:O	2.64	0.45
3:B:68:PHE:HA	3:B:71:PHE:CE2	2.50	0.45
3:M:167:LEU:O	3:M:171:TYR:N	2.49	0.45
1:C:452:LYS:HG3	1:R:452:LYS:CB	2.46	0.45
1:J:382:ARG:HH21	1:J:385:ILE:CD1	2.30	0.45
3:F:159:THR:CG2	3:F:162:PRO:CG	2.94	0.45
3:O:235:VAL:O	3:O:235:VAL:CG1	2.49	0.45
3:Q:48:ARG:CD	3:Q:48:ARG:H	2.29	0.45
1:L:320:SER:HB2	1:L:331:VAL:HG21	1.98	0.45
4:P:740:HOH:O	3:O:220:ARG:HD3	2.16	0.45
3:B:219:ARG:NH2	3:B:220:ARG:HD2	2.32	0.45
3:K:115:ALA:HB3	3:M:112:THR:CG2	2.46	0.45
3:M:62:PHE:HE2	4:M:932:HOH:O	1.99	0.45
3:Q:42:VAL:HG12	3:Q:188:LEU:CD1	2.46	0.45
3:M:59:ARG:NH1	3:M:215:ALA:HA	2.32	0.45
1:T:348:THR:HG22	1:T:350:ALA:H	1.81	0.45
2:V:398:LEU:HD12	2:V:398:LEU:N	2.32	0.45
1:J:358:LEU:HD23	1:J:386:MET:HE3	1.99	0.44
1:R:366:TYR:CD2	1:R:374:LEU:HD13	2.53	0.44
2:V:330:ASP:OD1	2:V:330:ASP:N	2.50	0.44
3:A:31:VAL:HG12	3:A:33:LEU:HD22	1.98	0.44
3:I:150:GLU:HG3	3:I:154:VAL:HG22	2.00	0.44
3:Q:207:SER:C	3:Q:208:LEU:HD23	2.37	0.44
3:S:45:ASN:OD1	3:S:45:ASN:C	2.56	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:W:56:LEU:HD13	3:W:99:LEU:HD22	2.00	0.44
3:Y:59:ARG:NH2	3:Y:217:ARG:O	2.46	0.44
1:P:362:GLU:OE2	1:P:382:ARG:HD3	2.17	0.44
3:K:181:LEU:HD23	3:K:233:LEU:HB3	1.98	0.44
3:O:20:ALA:O	3:O:24:ILE:HG13	2.17	0.44
3:O:182:ARG:NH2	3:O:234:LEU:O	2.50	0.44
3:Q:48:ARG:CD	3:Q:48:ARG:N	2.78	0.44
3:1:231:GLN:N	3:1:234:LEU:HD11	2.31	0.44
1:N:390:ASN:ND2	1:N:393:ALA:CB	2.78	0.44
1:P:382:ARG:NH2	1:P:385:ILE:CD1	2.76	0.44
3:K:159:THR:O	3:K:162:PRO:HD2	2.17	0.44
3:K:233:LEU:N	3:K:233:LEU:HD12	2.31	0.44
3:Q:52:LYS:HE3	3:Q:64:ALA:O	2.17	0.44
1:P:388:ARG:HG2	1:P:426:ALA:O	2.17	0.44
2:V:348:THR:CG2	2:V:351:VAL:CG1	2.96	0.44
3:I:142:THR:CG2	3:I:146:SER:HB2	2.47	0.44
3:K:233:LEU:N	3:K:233:LEU:CD1	2.80	0.44
3:W:71:PHE:CD1	3:W:71:PHE:C	2.91	0.44
1:C:383:LEU:O	1:C:387:VAL:HG23	2.17	0.44
1:N:424:ASP:OD1	1:N:427:GLY:N	2.50	0.44
3:D:103:TYR:HB2	3:D:141:ILE:HD12	2.00	0.44
3:U:129:HIS:HE1	4:U:250:HOH:O	1.99	0.44
3:W:109:THR:O	3:W:113:GLU:CB	2.65	0.44
3:I:30:VAL:HG13	3:I:43:ALA:HB2	2.00	0.44
1:P:307:LYS:HD3	4:P:541:HOH:O	2.17	0.44
1:T:465:ARG:HG3	1:T:513:LEU:HD22	1.99	0.44
3:A:45:ASN:C	3:A:207:SER:O	2.56	0.44
3:M:45:ASN:ND2	3:M:50:LEU:O	2.48	0.44
3:Q:18:GLU:OE2	3:Q:21:ARG:CZ	2.65	0.44
3:S:155:VAL:HG11	3:S:163:ILE:HB	2.00	0.44
1:H:320:SER:HB2	1:H:331:VAL:HG21	1.98	0.44
1:J:464:LEU:HD21	1:J:505:VAL:HG11	1.99	0.44
1:2:448:SER:HB3	4:2:543:HOH:O	2.18	0.44
3:A:142:THR:OG1	3:A:146:SER:HB2	2.18	0.44
3:U:163:ILE:HG12	3:U:191:GLY:H	1.82	0.44
3:U:232:ALA:HB2	4:U:592:HOH:O	2.17	0.44
1:N:359:TYR:CD1	1:N:386:MET:HE3	2.49	0.44
1:R:349:ALA:O	1:R:353:VAL:HG23	2.18	0.44
3:K:99:LEU:C	3:K:102:VAL:HG12	2.39	0.44
3:K:181:LEU:O	3:K:185:VAL:HG23	2.18	0.44
3:M:214:ASP:OD1	3:M:216:ASN:N	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:S:159:THR:CG2	3:S:162:PRO:HG2	2.47	0.44
1:C:382:ARG:HH21	1:C:385:ILE:HD13	1.81	0.43
1:L:391:LEU:HD12	1:L:391:LEU:C	2.32	0.43
1:T:348:THR:CB	1:T:351:VAL:HG12	2.45	0.43
1:T:492:PRO:O	1:T:510:ILE:HD13	2.18	0.43
1:X:319:ARG:HG3	1:X:320:SER:N	2.32	0.43
1:2:320:SER:HB2	1:2:331:VAL:HG21	1.99	0.43
3:F:111:PHE:HD1	3:F:117:PRO:HB3	1.82	0.43
3:F:217:ARG:HA	3:F:218:PRO:HD3	1.86	0.43
3:O:45:ASN:HA	3:O:46:PRO:HD3	1.72	0.43
3:Q:161:GLU:CB	3:Q:162:PRO:HD3	2.47	0.43
3:S:107:LEU:HD13	3:S:107:LEU:HA	1.85	0.43
1:2:374:LEU:HD11	3:U:89:TYR:HB3	2.00	0.43
3:A:28:LYS:HB3	3:A:44:GLU:HB3	2.00	0.43
3:A:35:TYR:CE1	3:A:37:GLY:N	2.86	0.43
3:I:141:ILE:HD12	3:I:141:ILE:N	2.34	0.43
3:I:203:LEU:N	3:I:203:LEU:CD1	2.80	0.43
3:O:59:ARG:HD2	3:O:129:HIS:HA	1.99	0.43
1:J:320:SER:HB2	1:J:331:VAL:HG21	2.00	0.43
1:R:301:OZT:C7	1:R:333:LYS:HZ1	2.25	0.43
2:G:354:GLU:CD	1:N:388:ARG:NH2	2.72	0.43
2:V:348:THR:CB	2:V:351:VAL:HG22	2.45	0.43
2:V:350:ALA:CB	1:2:428:GLY:HA3	2.48	0.43
3:D:217:ARG:HA	3:D:218:PRO:HD3	1.89	0.43
3:A:159:THR:HG22	3:A:162:PRO:CG	2.48	0.43
3:I:167:LEU:O	3:I:171:TYR:HB2	2.18	0.43
3:S:69:ASN:HD22	3:S:69:ASN:H	1.66	0.43
3:1:234:LEU:HD12	3:1:234:LEU:N	2.21	0.43
1:E:301:OZT:H17	1:E:333:LYS:HZ3	1.83	0.43
1:L:483:GLY:HA2	4:L:293:HOH:O	2.19	0.43
2:V:407:TYR:CE1	2:V:417:ALA:HB3	2.54	0.43
3:B:17:SER:HG	3:B:143:TYR:HE1	1.63	0.43
3:U:229:ALA:HB2	4:U:411:HOH:O	2.19	0.43
1:P:301:OZT:H27	1:P:333:LYS:HZ3	1.74	0.43
3:D:76:ARG:HD3	4:D:249:HOH:O	2.18	0.43
3:F:69:ASN:H	3:F:69:ASN:HD22	1.67	0.43
1:N:359:TYR:CA	1:N:386:MET:HE1	2.46	0.43
1:N:465:ARG:HG3	1:N:513:LEU:HD22	2.00	0.43
3:F:136:PRO:HG3	4:F:262:HOH:O	2.19	0.43
3:O:150:GLU:HA	3:O:151:PRO:HD3	1.82	0.43
3:Q:51:GLN:HB3	3:Q:209:GLU:OE2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:S:59:ARG:NH2	3:S:217:ARG:O	2.50	0.43
1:E:301:OZT:C7	1:E:333:LYS:NZ	2.82	0.43
2:G:338:ASP:OD2	2:G:379:LYS:HE2	2.19	0.43
1:T:383:LEU:O	1:T:387:VAL:HG23	2.19	0.43
1:Z:350:ALA:HA	1:Z:353:VAL:HG12	2.00	0.43
3:I:10:GLU:HB3	3:I:14:ARG:HH21	1.83	0.43
1:L:333:LYS:O	1:L:344:GLY:HA2	2.19	0.43
3:A:125:ALA:HB2	3:A:138:LEU:HD23	2.01	0.43
3:F:107:LEU:HD12	3:F:107:LEU:HA	1.85	0.43
3:F:142:THR:OG1	3:F:144:ASP:OD1	2.28	0.43
3:I:99:LEU:HA	3:I:102:VAL:HG12	2.01	0.43
3:W:72:ASP:O	3:W:76:ARG:HG3	2.19	0.43
3:Y:45:ASN:HA	3:Y:46:PRO:HD2	1.81	0.43
1:R:483:GLY:HA2	4:R:68:HOH:O	2.18	0.43
1:X:320:SER:HB2	1:X:331:VAL:HG21	2.01	0.43
1:X:330:ASP:OD1	1:X:490:ILE:CD1	2.63	0.43
3:I:48:ARG:H	3:I:48:ARG:HG2	1.51	0.43
3:K:54:SER:CB	3:K:75:ARG:HD2	2.49	0.43
3:S:59:ARG:HD2	3:S:128:ALA:O	2.18	0.43
1:L:301:OZT:C7	1:L:333:LYS:HZ1	2.28	0.42
1:N:423:PHE:CD2	1:N:423:PHE:N	2.87	0.42
1:T:348:THR:C	1:T:351:VAL:HG12	2.40	0.42
1:X:375:THR:HG21	3:Y:92:ARG:HG3	2.01	0.42
1:2:382:ARG:NH2	1:2:385:ILE:HD13	2.34	0.42
3:D:148:ALA:CB	4:D:603:HOH:O	2.67	0.42
3:A:114:GLN:HE21	3:A:114:GLN:HB3	1.63	0.42
3:B:219:ARG:HH22	3:B:220:ARG:HD2	1.84	0.42
3:Y:217:ARG:NH1	3:Y:220:ARG:O	2.52	0.42
1:H:382:ARG:HD2	3:B:89:TYR:HE1	1.84	0.42
1:R:320:SER:HB2	1:R:331:VAL:HG21	2.01	0.42
3:U:90:ASP:O	3:U:93:ASP:HB2	2.19	0.42
3:Y:129:HIS:O	3:Y:130:TYR:C	2.57	0.42
2:G:319:ARG:CG	2:G:320:SER:N	2.82	0.42
1:L:390:ASN:HD21	1:L:393:ALA:HB3	1.83	0.42
1:L:448:SER:HB3	1:P:448:SER:CB	2.48	0.42
1:N:415:GLN:HB3	4:N:905:HOH:O	2.19	0.42
3:D:85:ARG:HB3	3:D:93:ASP:OD1	2.20	0.42
3:F:44:GLU:OE1	3:F:188:LEU:CD2	2.67	0.42
3:1:231:GLN:OE1	3:1:234:LEU:HD13	2.18	0.42
1:E:363:LEU:HD12	1:E:363:LEU:HA	1.85	0.42
2:G:329:ARG:HD2	1:N:434:GLU:OE2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:35:TYR:HB2	3:K:175:ALA:O	2.19	0.42
3:K:99:LEU:O	3:K:102:VAL:HG13	2.18	0.42
3:Q:112:THR:CG2	3:Y:115:ALA:HB3	2.50	0.42
1:C:359:TYR:CE1	1:C:383:LEU:HB2	2.55	0.42
1:L:383:LEU:O	1:L:387:VAL:HG23	2.20	0.42
1:T:506:PRO:HD2	4:T:546:HOH:O	2.19	0.42
1:2:317:ASP:CG	1:2:333:LYS:HZ2	2.23	0.42
3:S:90:ASP:O	3:S:93:ASP:HB2	2.20	0.42
3:Y:41:PHE:HB3	3:Y:53:ILE:HD13	2.00	0.42
3:O:106:THR:O	3:O:110:ILE:HG13	2.20	0.42
1:L:348:THR:OG1	1:L:351:VAL:HG23	2.20	0.42
3:B:30:VAL:HG22	3:B:52:LYS:HE3	2.00	0.42
3:B:109:THR:O	3:B:113:GLU:HB2	2.20	0.42
3:M:95:THR:CG2	4:M:700:HOH:O	2.67	0.42
3:Q:150:GLU:HA	3:Q:151:PRO:HD2	1.75	0.42
3:U:70:GLU:HB3	3:U:118:TYR:CD2	2.54	0.42
3:Y:152:HIS:HB3	3:Y:171:TYR:CE2	2.54	0.42
1:C:301:OZT:H17	1:C:333:LYS:HZ1	1.66	0.42
1:C:366:TYR:CE2	1:C:374:LEU:HD13	2.54	0.42
2:G:465:ARG:HG3	2:G:513:LEU:HD22	2.02	0.42
3:B:67:LYS:HZ2	3:B:69:ASN:HD21	1.67	0.42
3:F:67:LYS:HG2	3:F:69:ASN:HD21	1.85	0.42
3:F:159:THR:HG22	3:F:159:THR:O	2.20	0.42
3:U:111:PHE:CD2	3:U:111:PHE:C	2.92	0.42
3:W:109:THR:O	3:W:113:GLU:HB2	2.20	0.42
1:P:366:TYR:CD2	1:P:374:LEU:HD13	2.54	0.42
1:R:319:ARG:CG	1:R:320:SER:N	2.83	0.42
1:2:353:VAL:O	1:2:357:ARG:HB2	2.20	0.42
3:B:159:THR:HG22	3:B:162:PRO:HD2	2.02	0.42
3:K:48:ARG:H	3:K:48:ARG:HG2	1.54	0.42
3:Y:54:SER:CB	3:Y:75:ARG:HD2	2.50	0.42
1:R:353:VAL:HG22	4:R:548:HOH:O	2.20	0.42
1:X:429:TRP:H	1:Z:350:ALA:HB2	1.85	0.42
3:Q:217:ARG:HA	4:Q:880:HOH:O	2.19	0.42
1:E:362:GLU:OE2	1:E:382:ARG:HD3	2.20	0.41
1:E:365:HIS:NE2	1:E:369:LEU:HD11	2.35	0.41
1:2:432:GLU:CD	1:2:437:GLN:HE21	2.23	0.41
3:B:176:SER:HB3	3:B:179:ASP:OD2	2.20	0.41
3:Q:181:LEU:CD1	3:Q:185:VAL:HG23	2.50	0.41
3:U:116:LYS:NZ	3:U:117:PRO:O	2.51	0.41
3:W:45:ASN:HA	3:W:46:PRO:HD2	1.97	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:444:LEU:HB2	4:H:30:HOH:O	2.19	0.41
1:E:382:ARG:HD2	3:K:89:TYR:HE1	1.83	0.41
1:T:319:ARG:CG	1:T:320:SER:N	2.83	0.41
1:T:319:ARG:NH1	1:T:479:SER:O	2.50	0.41
3:Q:161:GLU:H	3:Q:161:GLU:HG2	1.52	0.41
3:W:59:ARG:HD2	3:W:129:HIS:HA	2.01	0.41
1:H:301:OZT:C7	1:H:333:LYS:HE2	2.50	0.41
1:X:375:THR:OG1	3:Y:90:ASP:OD1	2.30	0.41
3:Q:59:ARG:HD2	3:Q:129:HIS:HA	2.01	0.41
1:T:353:VAL:HG13	1:T:354:GLU:N	2.35	0.41
2:V:319:ARG:CG	2:V:320:SER:N	2.83	0.41
3:B:56:LEU:HG	3:B:62:PHE:HB2	2.02	0.41
3:B:205:VAL:HG13	3:B:230:LEU:HD23	2.03	0.41
3:Q:44:GLU:HA	3:Q:208:LEU:HD22	2.03	0.41
3:Y:69:ASN:HD22	3:Y:69:ASN:H	1.68	0.41
1:C:444:LEU:HD12	1:C:444:LEU:HA	1.86	0.41
1:J:301:OZT:C7	1:J:333:LYS:NZ	2.76	0.41
1:J:366:TYR:OH	3:S:93:ASP:HB3	2.20	0.41
1:R:390:ASN:O	1:R:390:ASN:CG	2.59	0.41
3:D:52:LYS:HE3	3:D:64:ALA:O	2.20	0.41
3:F:18:GLU:OE1	3:F:22:LYS:CG	2.67	0.41
3:K:41:PHE:HE2	3:K:213:LEU:HG	1.86	0.41
3:S:210:VAL:CG1	3:S:211:ALA:N	2.83	0.41
3:U:181:LEU:CD2	4:U:747:HOH:O	2.68	0.41
3:1:45:ASN:HA	3:1:46:PRO:HD2	1.96	0.41
1:E:382:ARG:HH21	1:E:385:ILE:CD1	2.33	0.41
1:N:358:LEU:HD13	3:M:87:TYR:CZ	2.56	0.41
1:Z:319:ARG:O	1:Z:333:LYS:NZ	2.45	0.41
1:Z:382:ARG:HH21	1:Z:385:ILE:CD1	2.33	0.41
3:M:59:ARG:HD2	3:M:128:ALA:O	2.20	0.41
3:Q:179:ASP:O	3:Q:183:ILE:HD11	2.21	0.41
2:V:392:ALA:HB3	4:V:935:HOH:O	2.20	0.41
3:I:115:ALA:HB3	3:S:112:THR:HG23	2.03	0.41
3:1:116:LYS:HD2	3:1:117:PRO:O	2.20	0.41
1:C:382:ARG:HH21	1:C:385:ILE:CD1	2.33	0.41
1:L:355:PHE:CE2	1:L:383:LEU:HD11	2.55	0.41
1:N:354:GLU:OE2	1:N:354:GLU:HA	2.21	0.41
3:D:123:CYS:HA	3:D:139:TYR:O	2.20	0.41
3:A:56:LEU:HG	3:A:62:PHE:HB2	2.02	0.41
3:B:54:SER:CB	3:B:75:ARG:HD2	2.50	0.41
3:Y:163:ILE:HG23	3:Y:187:ALA:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:366:TYR:CG	2:G:374:LEU:HD13	2.55	0.41
2:V:337:THR:CG2	2:V:343:THR:OG1	2.69	0.41
2:V:348:THR:HG22	2:V:351:VAL:CB	2.39	0.41
1:Z:318:ARG:HD3	1:Z:493:THR:HG23	2.01	0.41
1:2:426:ALA:HB3	4:2:861:HOH:O	2.20	0.41
3:A:182:ARG:NH2	4:A:256:HOH:O	2.54	0.41
3:F:18:GLU:OE1	3:F:18:GLU:O	2.38	0.41
3:F:143:TYR:HD2	3:F:143:TYR:H	1.67	0.41
3:K:17:SER:O	3:K:21:ARG:HB2	2.21	0.41
3:M:55:GLU:HB2	3:M:222:PHE:CG	2.56	0.41
3:U:162:PRO:HB2	3:U:190:ALA:O	2.21	0.41
3:W:205:VAL:N	3:W:234:LEU:HD23	2.36	0.41
1:N:424:ASP:OD1	1:N:424:ASP:C	2.59	0.41
3:A:73:ASN:HD21	3:B:105:GLN:HG3	1.84	0.41
3:A:152:HIS:HB3	3:A:171:TYR:CE2	2.56	0.41
3:O:167:LEU:HG	3:O:187:ALA:CB	2.51	0.41
3:O:219:ARG:HD3	4:O:662:HOH:O	2.20	0.41
3:Q:56:LEU:HG	3:Q:62:PHE:HB2	2.03	0.41
3:Q:112:THR:HG23	3:Y:115:ALA:HB3	2.02	0.41
3:Y:107:LEU:HD13	3:Y:107:LEU:HA	1.94	0.41
1:L:382:ARG:CZ	1:L:385:ILE:HD12	2.52	0.40
3:M:214:ASP:OD1	3:M:214:ASP:C	2.60	0.40
1:C:358:LEU:HD23	1:C:386:MET:HE3	2.04	0.40
1:P:382:ARG:NH2	1:P:385:ILE:HD13	2.35	0.40
3:F:159:THR:O	3:F:162:PRO:HD2	2.21	0.40
3:M:181:LEU:O	3:M:185:VAL:HG23	2.22	0.40
3:Q:153:PHE:CD1	3:Q:153:PHE:C	2.94	0.40
3:S:116:LYS:HB2	3:I:112:THR:HG23	2.03	0.40
3:U:16:ARG:NH1	3:U:111:PHE:C	2.61	0.40
3:U:116:LYS:CE	3:U:119:GLU:OE1	2.69	0.40
3:W:67:LYS:HZ2	3:W:69:ASN:HD21	1.70	0.40
3:W:181:LEU:O	3:W:185:VAL:HG23	2.21	0.40
2:G:319:ARG:HG3	2:G:320:SER:N	2.36	0.40
1:T:429:TRP:N	1:2:350:ALA:HB2	2.36	0.40
1:Z:367:GLU:OE2	3:Y:220:ARG:NH2	2.54	0.40
3:I:159:THR:HG22	3:I:162:PRO:CG	2.52	0.40
3:M:54:SER:OG	3:M:55:GLU:N	2.55	0.40
3:O:45:ASN:N	3:O:207:SER:O	2.51	0.40
3:U:142:THR:HG23	4:U:859:HOH:O	2.21	0.40
1:N:376:PHE:CE2	1:N:380:ILE:HD11	2.56	0.40
1:Z:301:OZT:C7	1:Z:333:LYS:HZ1	2.30	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:115:ALA:HB3	3:K:112:THR:CG2	2.52	0.40
3:D:142:THR:OG1	3:D:146:SER:HB2	2.21	0.40
3:M:59:ARG:O	3:M:126:GLU:HA	2.22	0.40
3:O:18:GLU:O	3:O:22:LYS:HG3	2.22	0.40
3:W:144:ASP:OD1	3:W:144:ASP:N	2.54	0.40
3:Y:223:ARG:HA	4:Y:643:HOH:O	2.20	0.40
3:1:59:ARG:HD2	3:1:129:HIS:HA	2.04	0.40
1:L:366:TYR:CE2	1:L:374:LEU:HD13	2.57	0.40
1:Z:301:OZT:C7	1:Z:333:LYS:HZ3	2.23	0.40
1:Z:320:SER:HB2	1:Z:331:VAL:HG21	2.03	0.40
3:I:167:LEU:HD23	3:I:187:ALA:HB2	2.03	0.40
3:M:102:VAL:CG1	3:M:103:TYR:N	2.85	0.40
3:O:45:ASN:O	3:O:207:SER:HA	2.21	0.40
3:Q:41:PHE:O	3:Q:210:VAL:HG13	2.22	0.40
3:W:137:GLU:OE2	3:W:139:TYR:OH	2.30	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	2	220/240 (92%)	216 (98%)	4 (2%)	0	100	100
1	C	220/240 (92%)	218 (99%)	2 (1%)	0	100	100
1	E	220/240 (92%)	218 (99%)	2 (1%)	0	100	100
1	H	220/240 (92%)	216 (98%)	4 (2%)	0	100	100
1	J	220/240 (92%)	217 (99%)	3 (1%)	0	100	100
1	L	220/240 (92%)	218 (99%)	2 (1%)	0	100	100
1	N	220/240 (92%)	216 (98%)	4 (2%)	0	100	100
1	P	220/240 (92%)	218 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	R	220/240 (92%)	218 (99%)	1 (0%)	1 (0%)	29	52
1	T	220/240 (92%)	217 (99%)	3 (1%)	0	100	100
1	X	220/240 (92%)	217 (99%)	3 (1%)	0	100	100
1	Z	220/240 (92%)	217 (99%)	3 (1%)	0	100	100
2	G	220/240 (92%)	216 (98%)	4 (2%)	0	100	100
2	V	222/240 (92%)	219 (99%)	3 (1%)	0	100	100
3	1	209/240 (87%)	199 (95%)	9 (4%)	1 (0%)	29	52
3	A	210/240 (88%)	202 (96%)	8 (4%)	0	100	100
3	B	212/240 (88%)	205 (97%)	7 (3%)	0	100	100
3	D	209/240 (87%)	203 (97%)	6 (3%)	0	100	100
3	F	208/240 (87%)	203 (98%)	5 (2%)	0	100	100
3	I	213/240 (89%)	209 (98%)	4 (2%)	0	100	100
3	K	212/240 (88%)	206 (97%)	6 (3%)	0	100	100
3	M	190/240 (79%)	184 (97%)	6 (3%)	0	100	100
3	O	210/240 (88%)	204 (97%)	6 (3%)	0	100	100
3	Q	209/240 (87%)	202 (97%)	7 (3%)	0	100	100
3	S	211/240 (88%)	203 (96%)	8 (4%)	0	100	100
3	U	208/240 (87%)	201 (97%)	7 (3%)	0	100	100
3	W	205/240 (85%)	198 (97%)	7 (3%)	0	100	100
3	Y	209/240 (87%)	198 (95%)	11 (5%)	0	100	100
All	All	5997/6720 (89%)	5858 (98%)	137 (2%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	R	389	GLY
3	1	227	GLY

### 5.3.2 Protein sidechains [i](#)

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	2	164/177 (93%)	156 (95%)	8 (5%)	25	48
1	C	164/177 (93%)	149 (91%)	15 (9%)	9	18
1	E	164/177 (93%)	153 (93%)	11 (7%)	16	33
1	H	164/177 (93%)	151 (92%)	13 (8%)	12	24
1	J	164/177 (93%)	153 (93%)	11 (7%)	16	33
1	L	164/177 (93%)	155 (94%)	9 (6%)	21	43
1	N	164/177 (93%)	157 (96%)	7 (4%)	29	54
1	P	164/177 (93%)	154 (94%)	10 (6%)	18	38
1	R	164/177 (93%)	156 (95%)	8 (5%)	25	48
1	T	164/177 (93%)	157 (96%)	7 (4%)	29	54
1	X	164/177 (93%)	153 (93%)	11 (7%)	16	33
1	Z	164/177 (93%)	151 (92%)	13 (8%)	12	24
2	G	165/178 (93%)	158 (96%)	7 (4%)	30	55
2	V	165/178 (93%)	154 (93%)	11 (7%)	16	33
3	1	163/184 (89%)	152 (93%)	11 (7%)	16	33
3	A	164/184 (89%)	149 (91%)	15 (9%)	9	18
3	B	165/184 (90%)	155 (94%)	10 (6%)	18	38
3	D	163/184 (89%)	145 (89%)	18 (11%)	6	11
3	F	162/184 (88%)	143 (88%)	19 (12%)	5	10
3	I	166/184 (90%)	158 (95%)	8 (5%)	25	49
3	K	165/184 (90%)	153 (93%)	12 (7%)	14	28
3	M	148/184 (80%)	137 (93%)	11 (7%)	13	28
3	O	164/184 (89%)	155 (94%)	9 (6%)	21	43
3	Q	163/184 (89%)	150 (92%)	13 (8%)	12	24
3	S	165/184 (90%)	154 (93%)	11 (7%)	16	33
3	U	162/184 (88%)	152 (94%)	10 (6%)	18	37
3	W	160/184 (87%)	147 (92%)	13 (8%)	11	23
3	Y	163/184 (89%)	151 (93%)	12 (7%)	13	28
All	All	4571/5056 (90%)	4258 (93%)	313 (7%)	16	32

All (313) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	322	GLN
1	H	330	ASP
1	H	354	GLU
1	H	362	GLU
1	H	363	LEU
1	H	372	VAL
1	H	374	LEU
1	H	391	LEU
1	H	432	GLU
1	H	444	LEU
1	H	461	ASP
1	H	471	LEU
1	H	512	GLU
1	C	317	ASP
1	C	322	GLN
1	C	330	ASP
1	C	351	VAL
1	C	353	VAL
1	C	354	GLU
1	C	355	PHE
1	C	362	GLU
1	C	363	LEU
1	C	374	LEU
1	C	433	GLU
1	C	444	LEU
1	C	461	ASP
1	C	471	LEU
1	C	503	VAL
1	E	322	GLN
1	E	330	ASP
1	E	348	THR
1	E	362	GLU
1	E	363	LEU
1	E	374	LEU
1	E	433	GLU
1	E	444	LEU
1	E	461	ASP
1	E	471	LEU
1	E	519	GLU
2	G	322	GLN
2	G	362	GLU
2	G	363	LEU
2	G	444	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	G	461	ASP
2	G	471	LEU
2	G	512	GLU
1	J	322	GLN
1	J	330	ASP
1	J	348	THR
1	J	355	PHE
1	J	362	GLU
1	J	434	GLU
1	J	444	LEU
1	J	461	ASP
1	J	471	LEU
1	J	509	ARG
1	J	515	ARG
1	L	322	GLN
1	L	330	ASP
1	L	362	GLU
1	L	363	LEU
1	L	374	LEU
1	L	396	GLN
1	L	433	GLU
1	L	461	ASP
1	L	471	LEU
1	N	322	GLN
1	N	362	GLU
1	N	444	LEU
1	N	461	ASP
1	N	471	LEU
1	N	492	PRO
1	N	503	VAL
1	P	317	ASP
1	P	322	GLN
1	P	362	GLU
1	P	363	LEU
1	P	374	LEU
1	P	434	GLU
1	P	444	LEU
1	P	461	ASP
1	P	471	LEU
1	P	519	GLU
1	R	348	THR
1	R	362	GLU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	R	363	LEU
1	R	374	LEU
1	R	396	GLN
1	R	444	LEU
1	R	461	ASP
1	R	471	LEU
1	T	322	GLN
1	T	362	GLU
1	T	363	LEU
1	T	374	LEU
1	T	444	LEU
1	T	461	ASP
1	T	471	LEU
2	V	317	ASP
2	V	322	GLN
2	V	343	THR
2	V	363	LEU
2	V	412	SER
2	V	444	LEU
2	V	461	ASP
2	V	471	LEU
2	V	503	VAL
2	V	509	ARG
2	V	513	LEU
1	X	362	GLU
1	X	363	LEU
1	X	374	LEU
1	X	444	LEU
1	X	461	ASP
1	X	471	LEU
1	X	507	GLU
1	X	508	SER
1	X	509	ARG
1	X	513	LEU
1	X	519	GLU
1	Z	317	ASP
1	Z	322	GLN
1	Z	354	GLU
1	Z	362	GLU
1	Z	363	LEU
1	Z	374	LEU
1	Z	396	GLN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	Z	444	LEU
1	Z	461	ASP
1	Z	471	LEU
1	Z	507	GLU
1	Z	508	SER
1	Z	519	GLU
1	2	317	ASP
1	2	330	ASP
1	2	362	GLU
1	2	363	LEU
1	2	444	LEU
1	2	461	ASP
1	2	471	LEU
1	2	519	GLU
3	D	10	GLU
3	D	11	GLN
3	D	13	MET
3	D	21	ARG
3	D	69	ASN
3	D	73	ASN
3	D	74	LEU
3	D	90	ASP
3	D	93	ASP
3	D	102	VAL
3	D	113	GLU
3	D	114	GLN
3	D	133	THR
3	D	141	ILE
3	D	159	THR
3	D	169	GLU
3	D	188	LEU
3	D	234	LEU
3	A	9	MET
3	A	10	GLU
3	A	13	MET
3	A	21	ARG
3	A	33	LEU
3	A	73	ASN
3	A	74	LEU
3	A	102	VAL
3	A	107	LEU
3	A	170	SER

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
3	A	188	LEU
3	A	205	VAL
3	A	207	SER
3	A	208	LEU
3	A	216	ASN
3	B	17	SER
3	B	73	ASN
3	B	74	LEU
3	B	98	GLN
3	B	102	VAL
3	B	107	LEU
3	B	113	GLU
3	B	189	ARG
3	B	207	SER
3	B	216	ASN
3	F	13	MET
3	F	14	ARG
3	F	15	GLU
3	F	16	ARG
3	F	17	SER
3	F	18	GLU
3	F	21	ARG
3	F	73	ASN
3	F	74	LEU
3	F	90	ASP
3	F	102	VAL
3	F	107	LEU
3	F	113	GLU
3	F	116	LYS
3	F	168	LYS
3	F	188	LEU
3	F	192	SER
3	F	205	VAL
3	F	234	LEU
3	I	49	SER
3	I	69	ASN
3	I	73	ASN
3	I	74	LEU
3	I	107	LEU
3	I	142	THR
3	I	189	ARG
3	I	216	ASN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
3	K	11	GLN
3	K	13	MET
3	K	21	ARG
3	K	73	ASN
3	K	74	LEU
3	K	107	LEU
3	K	112	THR
3	K	113	GLU
3	K	132	GLU
3	K	169	GLU
3	K	188	LEU
3	K	216	ASN
3	M	62	PHE
3	M	74	LEU
3	M	102	VAL
3	M	105	GLN
3	M	107	LEU
3	M	113	GLU
3	M	159	THR
3	M	174	ASN
3	M	188	LEU
3	M	212	VAL
3	M	216	ASN
3	O	59	ARG
3	O	73	ASN
3	O	74	LEU
3	O	92	ARG
3	O	102	VAL
3	O	107	LEU
3	O	170	SER
3	O	188	LEU
3	O	233	LEU
3	Q	48	ARG
3	Q	73	ASN
3	Q	74	LEU
3	Q	102	VAL
3	Q	107	LEU
3	Q	113	GLU
3	Q	159	THR
3	Q	161	GLU
3	Q	173	GLU
3	Q	181	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
3	Q	188	LEU
3	Q	192	SER
3	Q	234	LEU
3	S	9	MET
3	S	73	ASN
3	S	74	LEU
3	S	92	ARG
3	S	102	VAL
3	S	107	LEU
3	S	188	LEU
3	S	192	SER
3	S	216	ASN
3	S	233	LEU
3	S	235	VAL
3	U	11	GLN
3	U	73	ASN
3	U	74	LEU
3	U	92	ARG
3	U	102	VAL
3	U	107	LEU
3	U	149	ASP
3	U	159	THR
3	U	169	GLU
3	U	212	VAL
3	W	42	VAL
3	W	74	LEU
3	W	99	LEU
3	W	107	LEU
3	W	140	ARG
3	W	159	THR
3	W	174	ASN
3	W	178	THR
3	W	179	ASP
3	W	188	LEU
3	W	205	VAL
3	W	216	ASN
3	W	233	LEU
3	Y	10	GLU
3	Y	11	GLN
3	Y	13	MET
3	Y	59	ARG
3	Y	73	ASN

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Mol	Chain	Res	Type
3	Y	74	LEU
3	Y	107	LEU
3	Y	113	GLU
3	Y	159	THR
3	Y	176	SER
3	Y	189	ARG
3	Y	207	SER
3	1	10	GLU
3	1	13	MET
3	1	21	ARG
3	1	73	ASN
3	1	74	LEU
3	1	102	VAL
3	1	107	LEU
3	1	113	GLU
3	1	159	THR
3	1	205	VAL
3	1	234	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (61) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	390	ASN
2	G	381	ASN
2	G	430	ASN
1	L	390	ASN
1	N	390	ASN
1	2	381	ASN
3	D	69	ASN
3	D	114	GLN
3	D	216	ASN
3	A	69	ASN
3	A	73	ASN
3	A	114	GLN
3	A	129	HIS
3	B	69	ASN
3	B	129	HIS
3	F	69	ASN
3	F	98	GLN
3	F	105	GLN
3	F	129	HIS
3	I	69	ASN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
3	I	73	ASN
3	I	129	HIS
3	K	69	ASN
3	K	73	ASN
3	K	129	HIS
3	K	231	GLN
3	M	69	ASN
3	M	98	GLN
3	M	105	GLN
3	M	114	GLN
3	M	174	ASN
3	M	216	ASN
3	M	231	GLN
3	O	69	ASN
3	O	73	ASN
3	O	129	HIS
3	O	231	GLN
3	Q	69	ASN
3	Q	114	GLN
3	S	69	ASN
3	S	73	ASN
3	S	98	GLN
3	S	105	GLN
3	S	174	ASN
3	U	69	ASN
3	U	129	HIS
3	U	152	HIS
3	W	69	ASN
3	W	80	GLN
3	W	98	GLN
3	W	114	GLN
3	W	152	HIS
3	W	174	ASN
3	Y	69	ASN
3	Y	73	ASN
3	Y	114	GLN
3	Y	174	ASN
3	1	11	GLN
3	1	69	ASN
3	1	73	ASN
3	1	98	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	OZT	L	301	1	7,9,10	5.09	5 (71%)	9,12,14	5.24	6 (66%)
1	OZT	J	301	1	7,9,10	4.61	5 (71%)	9,12,14	5.54	6 (66%)
1	OZT	T	301	1	7,9,10	5.26	6 (85%)	9,12,14	4.88	7 (77%)
1	OZT	H	301	1	7,9,10	5.26	6 (85%)	9,12,14	5.40	6 (66%)
1	OZT	R	301	1	7,9,10	5.08	5 (71%)	9,12,14	5.25	6 (66%)
1	OZT	Z	301	1	7,9,10	5.64	6 (85%)	9,12,14	4.81	6 (66%)
1	OZT	N	301	1	7,9,10	4.57	5 (71%)	9,12,14	5.01	7 (77%)
1	OZT	P	301	1	7,9,10	6.14	5 (71%)	9,12,14	5.78	7 (77%)
1	OZT	2	301	1	7,9,10	4.52	5 (71%)	9,12,14	4.95	6 (66%)
1	OZT	C	301	1	7,9,10	5.08	5 (71%)	9,12,14	5.25	6 (66%)
1	OZT	E	301	1	7,9,10	5.28	4 (57%)	9,12,14	5.24	7 (77%)
1	OZT	X	301	1	7,9,10	5.08	6 (85%)	9,12,14	5.17	7 (77%)

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
1	OZT	L	301	1	-	1/1/14/16	0/1/1/1
1	OZT	J	301	1	-	1/1/14/16	0/1/1/1
1	OZT	T	301	1	-	0/1/14/16	0/1/1/1
1	OZT	H	301	1	-	1/1/14/16	0/1/1/1
1	OZT	R	301	1	-	1/1/14/16	0/1/1/1

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

All (63) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	P	301	OZT	O1-C5	12.96	1.54	1.36
1	Z	301	OZT	O1-C5	12.58	1.53	1.36
1	E	301	OZT	O1-C5	11.43	1.52	1.36
1	H	301	OZT	O1-C5	11.26	1.51	1.36
1	J	301	OZT	O1-C5	10.57	1.50	1.36
1	X	301	OZT	O1-C5	10.45	1.50	1.36
1	L	301	OZT	O1-C5	10.38	1.50	1.36
1	R	301	OZT	O1-C5	10.38	1.50	1.36
1	C	301	OZT	O1-C5	10.34	1.50	1.36
1	T	301	OZT	O1-C5	10.14	1.50	1.36
1	2	301	OZT	O1-C5	10.10	1.50	1.36
1	N	301	OZT	C5-N	8.57	1.45	1.33
1	P	301	OZT	C5-N	7.23	1.43	1.33
1	T	301	OZT	C5-N	7.14	1.43	1.33
1	E	301	OZT	C5-N	6.67	1.43	1.33
1	L	301	OZT	C5-N	6.56	1.42	1.33
1	N	301	OZT	O1-C5	6.54	1.45	1.36
1	R	301	OZT	C5-N	6.54	1.42	1.33
1	C	301	OZT	C5-N	6.50	1.42	1.33
1	X	301	OZT	C5-N	6.47	1.42	1.33
1	Z	301	OZT	C5-N	5.17	1.40	1.33
1	H	301	OZT	C5-N	4.92	1.40	1.33
1	T	301	OZT	O6-C5	4.30	1.29	1.21
1	H	301	OZT	O1-C2	-4.28	1.40	1.46
1	C	301	OZT	O1-C2	-4.14	1.40	1.46
1	Z	301	OZT	O1-C2	-4.13	1.40	1.46
1	L	301	OZT	O1-C2	-4.10	1.40	1.46
1	R	301	OZT	O1-C2	-4.05	1.40	1.46
1	P	301	OZT	O6-C5	3.94	1.29	1.21
1	J	301	OZT	O1-C2	-3.79	1.41	1.46
1	P	301	OZT	C2-CA	-3.73	1.47	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	N	301	OZT	O1-C2	-3.64	1.41	1.46
1	2	301	OZT	O1-C2	-3.62	1.41	1.46
1	T	301	OZT	O1-C2	-3.57	1.41	1.46
1	H	301	OZT	C7-C2	-3.55	1.43	1.51
1	X	301	OZT	O1-C2	-3.49	1.41	1.46
1	2	301	OZT	C2-CA	-3.24	1.48	1.54
1	2	301	OZT	C5-N	3.23	1.38	1.33
1	J	301	OZT	C5-N	3.23	1.38	1.33
1	P	301	OZT	O1-C2	-3.22	1.41	1.46
1	Z	301	OZT	O6-C5	3.02	1.27	1.21
1	N	301	OZT	O6-C5	2.67	1.26	1.21
1	X	301	OZT	C2-CA	-2.64	1.49	1.54
1	N	301	OZT	C7-C2	-2.62	1.45	1.51
1	H	301	OZT	C2-CA	-2.60	1.49	1.54
1	C	301	OZT	C7-C2	-2.57	1.45	1.51
1	L	301	OZT	C7-C2	-2.57	1.45	1.51
1	R	301	OZT	C7-C2	-2.56	1.45	1.51
1	J	301	OZT	C7-C2	-2.54	1.45	1.51
1	E	301	OZT	O6-C5	2.52	1.26	1.21
1	E	301	OZT	C2-CA	-2.49	1.49	1.54
1	Z	301	OZT	C2-CA	-2.47	1.49	1.54
1	X	301	OZT	O6-C5	2.42	1.26	1.21
1	J	301	OZT	C2-CA	-2.19	1.50	1.54
1	Z	301	OZT	C7-C2	-2.16	1.46	1.51
1	H	301	OZT	O6-C5	2.13	1.25	1.21
1	C	301	OZT	O6-C5	2.13	1.25	1.21
1	T	301	OZT	C2-CA	-2.12	1.50	1.54
1	R	301	OZT	O6-C5	2.10	1.25	1.21
1	L	301	OZT	O6-C5	2.09	1.25	1.21
1	T	301	OZT	C7-C2	-2.05	1.46	1.51
1	X	301	OZT	C7-C2	-2.03	1.46	1.51
1	2	301	OZT	C7-C2	-2.03	1.46	1.51

All (77) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	301	OZT	O1-C5-N	9.29	117.65	109.86
1	P	301	OZT	O1-C2-CA	8.91	112.17	103.58
1	R	301	OZT	O1-C5-N	8.48	116.97	109.86
1	C	301	OZT	O1-C5-N	8.47	116.97	109.86
1	L	301	OZT	O1-C5-N	8.43	116.94	109.86
1	H	301	OZT	O1-C5-N	8.39	116.90	109.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	301	OZT	O1-C5-N	8.33	116.85	109.86
1	T	301	OZT	O1-C2-CA	8.25	111.53	103.58
1	N	301	OZT	O1-C5-N	8.01	116.58	109.86
1	X	301	OZT	O1-C2-CA	7.87	111.17	103.58
1	X	301	OZT	O1-C5-N	7.85	116.44	109.86
1	E	301	OZT	O1-C5-N	7.83	116.43	109.86
1	N	301	OZT	O1-C2-CA	7.73	111.03	103.58
1	J	301	OZT	O6-C5-N	-7.52	120.43	129.22
1	E	301	OZT	O1-C2-CA	7.43	110.75	103.58
1	P	301	OZT	C2-O1-C5	-7.32	98.44	110.41
1	Z	301	OZT	O1-C5-N	7.24	115.93	109.86
1	P	301	OZT	O1-C5-N	7.22	115.92	109.86
1	T	301	OZT	O1-C5-N	6.98	115.72	109.86
1	E	301	OZT	C2-O1-C5	-6.91	99.10	110.41
1	C	301	OZT	O1-C2-CA	6.85	110.19	103.58
1	H	301	OZT	O1-C2-CA	6.84	110.18	103.58
1	R	301	OZT	O1-C2-CA	6.82	110.16	103.58
1	L	301	OZT	O1-C2-CA	6.81	110.15	103.58
1	2	301	OZT	O6-C5-N	-6.77	121.31	129.22
1	H	301	OZT	C2-CA-C	-6.73	104.80	114.16
1	R	301	OZT	C2-CA-C	-6.71	104.83	114.16
1	L	301	OZT	C2-CA-C	-6.70	104.84	114.16
1	C	301	OZT	C2-CA-C	-6.70	104.85	114.16
1	X	301	OZT	C2-O1-C5	-6.64	99.55	110.41
1	J	301	OZT	C2-O1-C5	-6.63	99.57	110.41
1	H	301	OZT	C2-O1-C5	-6.58	99.64	110.41
1	H	301	OZT	O6-C5-N	-6.48	121.65	129.22
1	P	301	OZT	O6-C5-N	-6.41	121.73	129.22
1	Z	301	OZT	O1-C2-CA	6.30	109.66	103.58
1	J	301	OZT	O1-C2-CA	6.29	109.65	103.58
1	T	301	OZT	C2-O1-C5	-6.27	100.15	110.41
1	Z	301	OZT	O6-C5-N	-6.26	121.90	129.22
1	E	301	OZT	O6-C5-N	-6.25	121.91	129.22
1	Z	301	OZT	C2-O1-C5	-6.21	100.25	110.41
1	R	301	OZT	C2-O1-C5	-6.15	100.34	110.41
1	2	301	OZT	C2-O1-C5	-6.13	100.37	110.41
1	C	301	OZT	C2-O1-C5	-6.13	100.38	110.41
1	L	301	OZT	C2-O1-C5	-6.12	100.39	110.41
1	P	301	OZT	C2-CA-C	-5.94	105.90	114.16
1	2	301	OZT	O1-C2-CA	5.94	109.31	103.58
1	N	301	OZT	C2-CA-C	-5.92	105.93	114.16
1	P	301	OZT	C7-C2-CA	-5.82	106.62	114.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	R	301	OZT	O6-C5-N	-5.67	122.59	129.22
1	X	301	OZT	O6-C5-N	-5.66	122.60	129.22
1	C	301	OZT	O6-C5-N	-5.64	122.63	129.22
1	L	301	OZT	O6-C5-N	-5.64	122.63	129.22
1	N	301	OZT	C2-O1-C5	-5.61	101.23	110.41
1	J	301	OZT	C2-CA-C	-5.55	106.44	114.16
1	T	301	OZT	O6-C5-N	-5.05	123.33	129.22
1	Z	301	OZT	C2-CA-C	-4.75	107.55	114.16
1	E	301	OZT	C2-CA-C	-4.57	107.81	114.16
1	X	301	OZT	C2-CA-C	-4.42	108.02	114.16
1	2	301	OZT	C2-CA-C	-4.32	108.15	114.16
1	E	301	OZT	C7-C2-CA	-4.27	108.79	114.80
1	T	301	OZT	C2-CA-C	-4.18	108.34	114.16
1	X	301	OZT	C7-C2-CA	-3.95	109.25	114.80
1	J	301	OZT	C7-C2-CA	-3.91	109.31	114.80
1	Z	301	OZT	C7-C2-CA	-3.57	109.77	114.80
1	N	301	OZT	O1-C5-O6	-3.42	117.76	121.24
1	H	301	OZT	C7-C2-CA	-3.38	110.04	114.80
1	N	301	OZT	O6-C5-N	-3.36	125.30	129.22
1	C	301	OZT	C7-C2-CA	-3.34	110.10	114.80
1	L	301	OZT	C7-C2-CA	-3.32	110.13	114.80
1	R	301	OZT	C7-C2-CA	-3.32	110.13	114.80
1	2	301	OZT	C7-C2-CA	-3.23	110.25	114.80
1	T	301	OZT	C7-C2-CA	-3.20	110.30	114.80
1	N	301	OZT	C7-C2-CA	-2.76	110.92	114.80
1	X	301	OZT	O-C-CA	-2.37	118.22	124.83
1	E	301	OZT	O-C-CA	-2.13	118.90	124.83
1	T	301	OZT	O-C-CA	-2.07	119.05	124.83
1	P	301	OZT	O-C-CA	-2.05	119.11	124.83

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	H	301	OZT	O-C-CA-C2
1	C	301	OZT	O-C-CA-C2
1	E	301	OZT	O-C-CA-C2
1	J	301	OZT	O-C-CA-C2
1	L	301	OZT	O-C-CA-C2
1	P	301	OZT	O-C-CA-C2
1	R	301	OZT	O-C-CA-C2
1	Z	301	OZT	O-C-CA-C2

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Mol	Chain	Res	Type	Atoms
1	2	301	OZT	O-C-CA-C2

There are no ring outliers.

12 monomers are involved in 67 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	L	301	OZT	5	0
1	J	301	OZT	5	0
1	T	301	OZT	6	0
1	H	301	OZT	6	0
1	R	301	OZT	5	0
1	Z	301	OZT	7	0
1	N	301	OZT	3	0
1	P	301	OZT	7	0
1	2	301	OZT	5	0
1	C	301	OZT	6	0
1	E	301	OZT	5	0
1	X	301	OZT	7	0

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data i

### 6.1 Protein, DNA and RNA chains i

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	2	221/240 (92%)	-0.39	3 (1%) 75 71	14, 40, 80, 106	0
1	C	221/240 (92%)	-0.24	7 (3%) 47 40	16, 46, 84, 106	0
1	E	221/240 (92%)	-0.25	5 (2%) 60 54	22, 45, 81, 114	0
1	H	221/240 (92%)	-0.34	5 (2%) 60 54	14, 37, 86, 102	0
1	J	221/240 (92%)	-0.28	4 (1%) 68 64	17, 45, 86, 111	0
1	L	221/240 (92%)	-0.43	7 (3%) 47 40	10, 37, 82, 110	0
1	N	221/240 (92%)	-0.44	11 (4%) 28 23	6, 28, 85, 120	0
1	P	221/240 (92%)	-0.45	4 (1%) 68 64	10, 29, 78, 109	0
1	R	221/240 (92%)	-0.28	4 (1%) 68 64	21, 48, 89, 115	0
1	T	221/240 (92%)	-0.22	9 (4%) 37 30	12, 42, 84, 120	0
1	X	221/240 (92%)	-0.20	10 (4%) 33 26	16, 38, 80, 116	0
1	Z	221/240 (92%)	-0.10	10 (4%) 33 26	21, 48, 84, 111	0
2	G	222/240 (92%)	-0.36	3 (1%) 75 71	11, 45, 79, 109	0
2	V	224/240 (93%)	-0.47	4 (1%) 68 64	9, 30, 79, 108	0
3	1	213/240 (88%)	0.65	30 (14%) 2 1	27, 70, 104, 115	0
3	A	214/240 (89%)	-0.28	1 (0%) 91 89	7, 45, 85, 101	0
3	B	216/240 (90%)	-0.28	1 (0%) 91 89	6, 40, 85, 102	0
3	D	213/240 (88%)	0.38	17 (7%) 12 9	19, 70, 102, 125	0
3	F	212/240 (88%)	0.07	13 (6%) 21 16	16, 55, 128, 161	0
3	I	217/240 (90%)	-0.27	1 (0%) 91 89	15, 44, 83, 101	0
3	K	216/240 (90%)	0.06	1 (0%) 91 89	18, 60, 94, 115	0
3	M	194/240 (80%)	0.81	37 (19%) 1 0	26, 73, 103, 116	0
3	O	214/240 (89%)	-0.15	3 (1%) 75 71	16, 55, 93, 106	0
3	Q	213/240 (88%)	0.55	29 (13%) 3 1	27, 70, 108, 130	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
3	S	215/240 (89%)	0.04	5 (2%) 60 54	17, 56, 95, 113	0
3	U	212/240 (88%)	0.90	36 (16%) 1 1	20, 76, 105, 120	0
3	W	209/240 (87%)	0.40	18 (8%) 10 7	25, 66, 99, 112	0
3	Y	213/240 (88%)	0.09	8 (3%) 40 33	19, 62, 97, 114	0
All	All	6069/6720 (90%)	-0.06	286 (4%) 31 25	6, 49, 95, 161	0

All (286) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	X	425	ALA	7.2
3	M	192	SER	7.0
1	N	398	LEU	6.9
1	E	398	LEU	6.6
3	M	158	GLY	6.6
3	1	36	ALA	6.2
3	M	159	THR	6.0
3	Q	169	GLU	6.0
1	N	395	MET	5.9
3	D	11	GLN	5.9
1	Z	397	GLY	5.9
3	U	227	GLY	5.8
1	X	395	MET	5.7
3	Y	205	VAL	5.6
3	Q	192	SER	5.2
3	1	188	LEU	5.1
3	U	169	GLU	5.1
3	1	183	ILE	5.0
1	X	397	GLY	5.0
1	N	394	ALA	4.9
3	U	10	GLU	4.9
1	J	395	MET	4.9
1	T	396	GLN	4.9
1	T	350	ALA	4.9
1	N	392	ALA	4.9
3	U	165	ASN	4.9
1	T	397	GLY	4.8
2	V	349	ALA	4.8
1	N	396	GLN	4.8
1	E	396	GLN	4.7
3	Q	225	ILE	4.7
3	1	191	GLY	4.7

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
3	F	15	GLU	4.6
3	M	230	LEU	4.6
1	Z	392	ALA	4.6
3	M	169	GLU	4.5
1	X	398	LEU	4.5
3	Q	234	LEU	4.5
1	L	395	MET	4.5
3	U	160	THR	4.4
3	U	231	GLN	4.4
3	W	208	LEU	4.4
3	U	188	LEU	4.3
3	M	191	GLY	4.3
3	U	11	GLN	4.3
3	1	169	GLU	4.2
3	Y	169	GLU	4.0
3	M	188	LEU	4.0
3	F	13	MET	4.0
1	R	398	LEU	4.0
3	U	181	LEU	4.0
3	W	191	GLY	4.0
3	U	186	ALA	4.0
3	U	180	ALA	3.9
1	X	396	GLN	3.9
3	1	172	ALA	3.9
1	2	395	MET	3.9
3	W	205	VAL	3.9
3	W	169	GLU	3.9
1	J	396	GLN	3.8
3	M	190	ALA	3.8
1	N	397	GLY	3.8
3	M	165	ASN	3.8
3	Y	234	LEU	3.8
3	M	189	ARG	3.8
3	W	113	GLU	3.8
1	E	395	MET	3.8
3	U	230	LEU	3.7
3	U	162	PRO	3.7
3	U	167	LEU	3.7
3	M	181	LEU	3.7
3	U	163	ILE	3.6
3	U	184	ALA	3.6
3	F	11	GLN	3.6

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	T	398	LEU	3.6
3	U	205	VAL	3.6
3	D	165	ASN	3.6
1	N	425	ALA	3.5
3	W	114	GLN	3.5
1	N	427	GLY	3.5
3	D	10	GLU	3.5
3	F	16	ARG	3.5
1	H	347	GLY	3.4
1	N	400	ALA	3.4
1	T	349	ALA	3.4
3	Q	36	ALA	3.4
1	X	399	LEU	3.4
3	F	21	ARG	3.4
1	Z	398	LEU	3.4
3	F	18	GLU	3.3
3	Q	113	GLU	3.3
3	Q	231	GLN	3.3
1	T	348	THR	3.3
3	U	164	ALA	3.3
3	1	133	THR	3.3
1	R	396	GLN	3.3
3	1	171	TYR	3.3
3	1	12	ALA	3.2
1	L	396	GLN	3.2
3	Q	188	LEU	3.2
3	U	233	LEU	3.2
3	U	157	GLY	3.2
3	K	192	SER	3.2
1	2	397	GLY	3.2
1	J	392	ALA	3.2
1	L	398	LEU	3.2
3	1	173	GLU	3.1
3	W	192	SER	3.1
3	1	192	SER	3.1
3	M	115	ALA	3.1
3	1	19	LEU	3.1
3	U	225	ILE	3.1
3	1	159	THR	3.0
1	R	395	MET	3.0
1	L	397	GLY	3.0
3	W	159	THR	3.0

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
3	D	232	ALA	3.0
3	U	179	ASP	3.0
3	W	233	LEU	3.0
1	2	392	ALA	3.0
3	D	190	ALA	3.0
3	F	115	ALA	3.0
3	F	22	LYS	3.0
3	Q	232	ALA	3.0
2	V	348	THR	2.9
3	Q	172	ALA	2.9
3	Q	173	GLU	2.9
3	Y	191	GLY	2.9
3	M	208	LEU	2.9
3	W	180	ALA	2.9
3	Q	227	GLY	2.9
3	D	231	GLN	2.9
3	W	234	LEU	2.9
3	1	13	MET	2.9
1	L	425	ALA	2.9
3	1	48	ARG	2.9
3	M	116	LYS	2.9
3	1	167	LEU	2.8
3	M	133	THR	2.8
3	U	159	THR	2.8
3	U	154	VAL	2.8
3	W	20	ALA	2.8
3	1	227	GLY	2.8
3	U	33	LEU	2.8
1	X	393	ALA	2.8
3	1	135	ARG	2.8
3	U	24	ILE	2.8
1	H	393	ALA	2.8
1	C	395	MET	2.8
1	N	393	ALA	2.7
1	T	395	MET	2.7
2	V	396	GLN	2.7
1	P	353	VAL	2.7
3	Q	205	VAL	2.7
3	U	191	GLY	2.7
3	W	115	ALA	2.7
3	1	182	ARG	2.7
3	U	158	GLY	2.7

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
3	F	14	ARG	2.7
3	1	26	ARG	2.7
1	Z	412	SER	2.7
1	C	397	GLY	2.6
1	L	394	ALA	2.6
3	U	226	THR	2.6
3	M	27	ALA	2.6
3	D	160	THR	2.6
1	P	395	MET	2.6
3	W	182	ARG	2.6
1	X	394	ALA	2.6
3	Q	10	GLU	2.6
1	Z	391	LEU	2.6
3	O	19	LEU	2.6
1	T	415	GLN	2.6
3	D	113	GLU	2.6
1	X	426	ALA	2.6
1	P	396	GLN	2.6
3	D	131	GLY	2.6
3	Y	182	ARG	2.6
3	M	117	PRO	2.6
1	E	425	ALA	2.6
3	Q	233	LEU	2.5
3	M	207	SER	2.5
1	X	392	ALA	2.5
3	D	186	ALA	2.5
3	U	228	SER	2.5
1	J	349	ALA	2.5
1	R	400	ALA	2.5
3	W	110	ILE	2.5
3	Q	130	TYR	2.5
3	D	191	GLY	2.5
1	H	395	MET	2.5
3	Y	26	ARG	2.5
1	Z	425	ALA	2.5
3	O	205	VAL	2.5
3	D	13	MET	2.5
3	U	112	THR	2.5
3	Q	160	THR	2.4
3	M	131	GLY	2.4
3	M	162	PRO	2.4
3	Q	230	LEU	2.4

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
3	M	114	GLN	2.4
2	V	350	ALA	2.4
3	Y	233	LEU	2.4
3	1	175	ALA	2.4
3	F	169	GLU	2.4
3	W	39	VAL	2.4
3	Q	131	GLY	2.4
1	L	392	ALA	2.4
3	W	232	ALA	2.4
1	E	347	GLY	2.4
3	1	174	ASN	2.4
3	U	177	LEU	2.4
3	F	131	GLY	2.4
3	M	216	ASN	2.4
3	D	164	ALA	2.3
3	M	232	ALA	2.3
3	1	179	ASP	2.3
3	A	231	GLN	2.3
2	G	426	ALA	2.3
1	Z	395	MET	2.3
1	T	392	ALA	2.3
3	1	37	GLY	2.3
3	Q	159	THR	2.3
3	1	165	ASN	2.3
3	1	153	PHE	2.3
3	M	111	PHE	2.3
3	B	182	ARG	2.3
3	M	48	ARG	2.3
3	Q	135	ARG	2.3
1	H	349	ALA	2.3
3	U	170	SER	2.3
1	H	396	GLN	2.3
1	Z	426	ALA	2.3
3	1	15	GLU	2.3
1	C	409	ILE	2.3
1	C	413	ASP	2.3
3	Q	191	GLY	2.2
1	C	398	LEU	2.2
3	F	113	GLU	2.2
3	Q	133	THR	2.2
3	1	22	LYS	2.2
3	D	205	VAL	2.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	C	350	ALA	2.2
3	Q	12	ALA	2.2
3	U	183	ILE	2.2
3	M	113	GLU	2.2
3	M	229	ALA	2.2
3	I	48	ARG	2.2
3	M	157	GLY	2.2
3	M	163	ILE	2.2
3	F	232	ALA	2.2
1	Z	396	GLN	2.2
2	G	396	GLN	2.2
1	P	425	ALA	2.2
3	U	166	ALA	2.2
3	S	133	THR	2.2
3	D	14	ARG	2.2
3	O	235	VAL	2.1
3	D	21	ARG	2.1
3	M	184	ALA	2.1
3	S	161	GLU	2.1
3	M	46	PRO	2.1
3	Q	33	LEU	2.1
3	M	67	LYS	2.1
2	G	347	GLY	2.1
3	Y	171	TYR	2.1
3	D	161	GLU	2.1
1	C	392	ALA	2.1
3	S	36	ALA	2.1
3	M	176	SER	2.1
3	M	144	ASP	2.1
3	Q	210	VAL	2.1
3	Q	229	ALA	2.1
1	Z	399	LEU	2.1
3	Q	189	ARG	2.1
3	S	9	MET	2.1
3	Q	177	LEU	2.0
3	M	143	TYR	2.0
3	U	216	ASN	2.0
3	W	184	ALA	2.0
3	I	170	SER	2.0
3	S	167	LEU	2.0
1	N	428	GLY	2.0
3	M	206	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
3	M	123	CYS	2.0
3	1	150	GLU	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
1	OZT	Z	301	9/10	0.84	0.22	36,41,47,48	0
1	OZT	T	301	9/10	0.88	0.24	31,38,44,46	0
1	OZT	C	301	9/10	0.89	0.23	72,76,77,78	0
1	OZT	P	301	9/10	0.89	0.18	34,41,46,47	0
1	OZT	R	301	9/10	0.90	0.17	63,65,66,68	0
1	OZT	H	301	9/10	0.91	0.18	35,41,45,46	0
1	OZT	E	301	9/10	0.91	0.19	36,42,46,48	0
1	OZT	X	301	9/10	0.92	0.14	24,28,31,32	0
1	OZT	2	301	9/10	0.92	0.14	31,34,39,43	0
1	OZT	L	301	9/10	0.93	0.15	27,33,36,37	0
1	OZT	J	301	9/10	0.94	0.12	34,38,40,41	0
1	OZT	N	301	9/10	0.96	0.13	23,26,31,32	0

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.