Full wwPDB X-ray Structure Validation Report ⓘ

May 3, 2025 – 02:24 PM EDT

PDB ID	:	3MFE / pdb_00003mfe
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*
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.

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

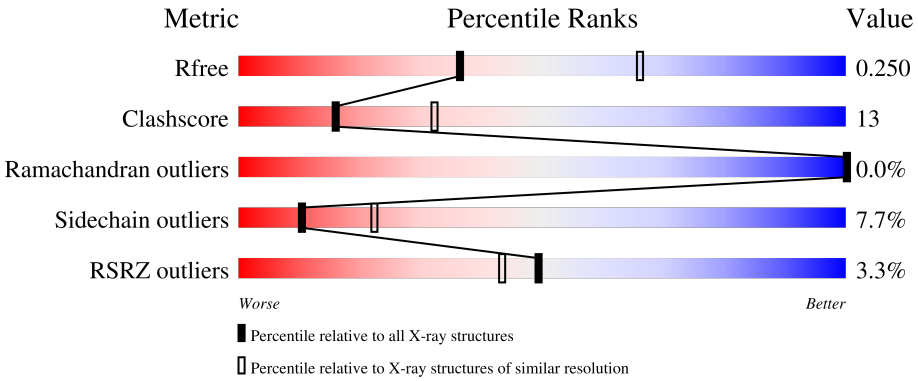
MolProbity	:	4-5-2 with Phenix2.0rc1
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

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}	164625	3775 (2.60-2.60)
Clashscore	180529	4181 (2.60-2.60)
Ramachandran outliers	177936	4129 (2.60-2.60)
Sidechain outliers	177891	4129 (2.60-2.60)
RSRZ outliers	164620	3775 (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 >=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 <=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	79% 12% • 8%
1	C	240	2% 73% 17% • 8%
1	E	240	% 75% 15% • 8%
1	H	240	2% 77% 12% • 8%
1	J	240	2% 78% 12% • 8%

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Mol	Chain	Length	Quality of chain
1	L	240	75% 17% 8%
1	N	240	70% 21% 8%
1	P	240	3% 76% 14% 8%
1	R	240	73% 16% 8%
1	T	240	74% 18% 8%
1	X	240	77% 12% 8%
1	Z	240	77% 14% 8%
2	G	240	74% 17% 8%
2	V	240	3% 70% 21% 7%
3	1	240	5% 74% 14% 11%
3	A	240	66% 19% 11%
3	B	240	3% 64% 23% 10%
3	D	240	5% 64% 22% 11%
3	F	240	7% 59% 21% 9% 12%
3	I	240	65% 22% 10%
3	K	240	62% 24% 10%
3	M	240	5% 54% 23% 19%
3	O	240	3% 63% 22% 11%
3	Q	240	7% 58% 26% 11%
3	S	240	67% 19% 10%
3	U	240	16% 58% 30% 12%
3	W	240	57% 28% 13%
3	Y	240	58% 28% 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
1	H	222	Total	C	N	O	S	0	0	0
			1640	1028	282	325	5			
1	C	222	Total	C	N	O	S	0	0	0
			1640	1028	282	325	5			
1	E	222	Total	C	N	O	S	0	0	0
			1640	1028	282	325	5			
1	J	222	Total	C	N	O	S	0	0	0
			1640	1028	282	325	5			
1	L	222	Total	C	N	O	S	0	0	0
			1640	1028	282	325	5			
1	N	222	Total	C	N	O	S	0	0	0
			1640	1028	282	325	5			
1	P	222	Total	C	N	O	S	0	0	0
			1640	1028	282	325	5			
1	R	222	Total	C	N	O	S	0	0	0
			1640	1028	282	325	5			
1	T	222	Total	C	N	O	S	0	0	0
			1640	1028	282	325	5			
1	X	222	Total	C	N	O	S	0	0	0
			1640	1028	282	325	5			
1	Z	222	Total	C	N	O	S	0	0	0
			1640	1028	282	325	5			
1	2	222	Total	C	N	O	S	0	0	0
			1640	1028	282	325	5			

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
2	G	222	Total	C	N	O	S	0	0	0
			1638	1027	282	324	5			

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

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

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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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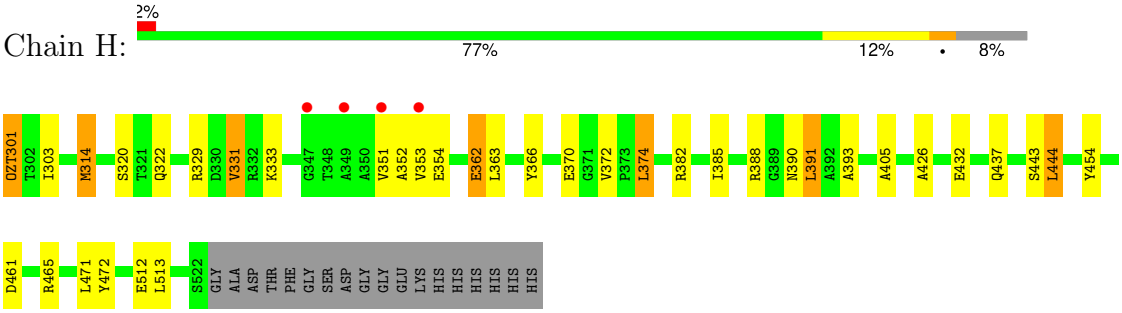
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	1	22	Total O 22 22	0	0

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.

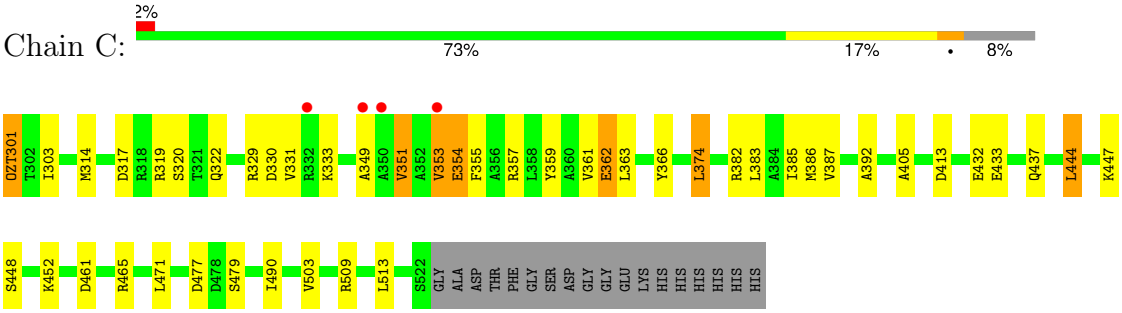
• Molecule 1: Proteasome subunit beta

Chain H:



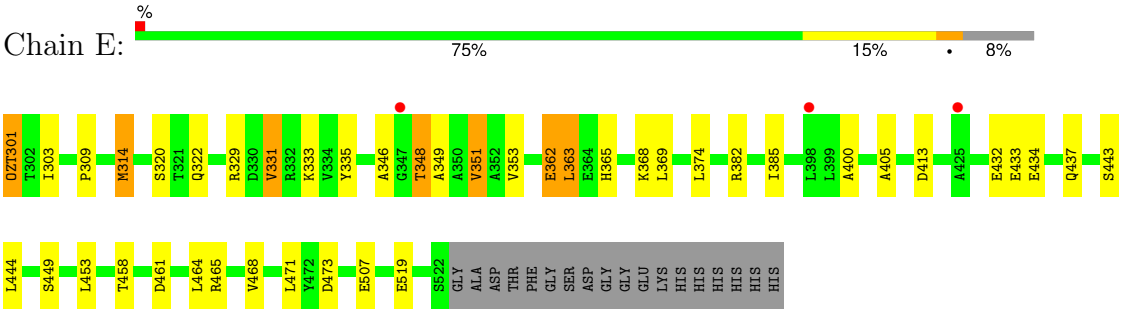
• Molecule 1: Proteasome subunit beta

Chain C:



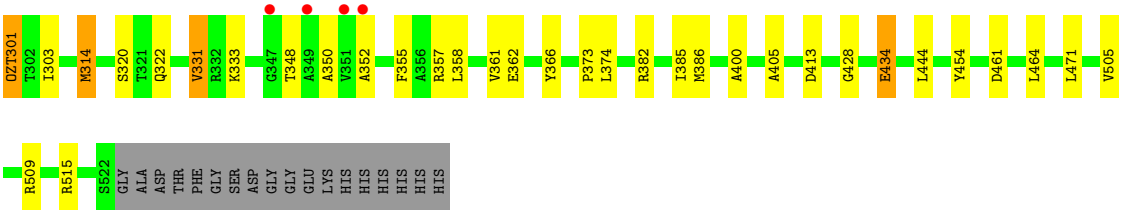
• Molecule 1: Proteasome subunit beta

Chain E:



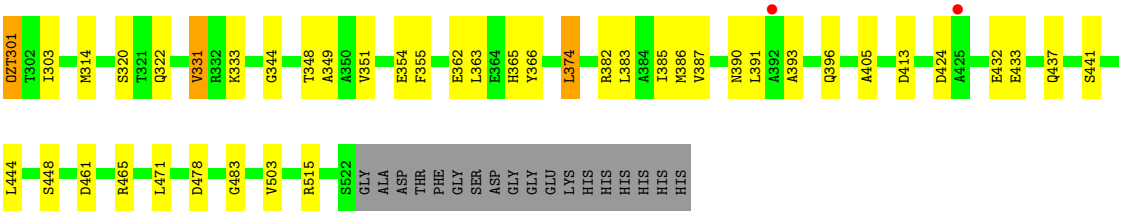
• Molecule 1: Proteasome subunit beta

Chain J:



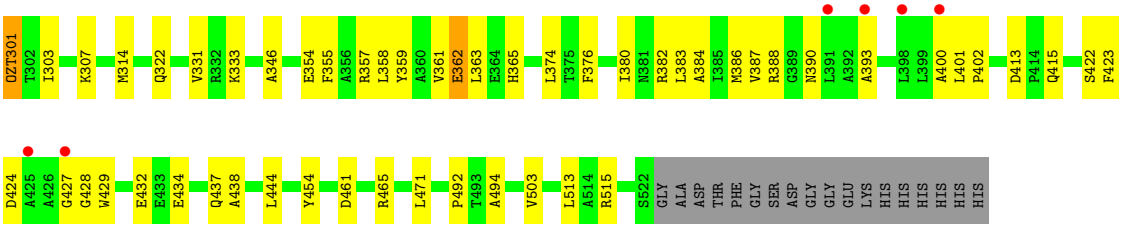
• Molecule 1: Proteasome subunit beta

Chain L:



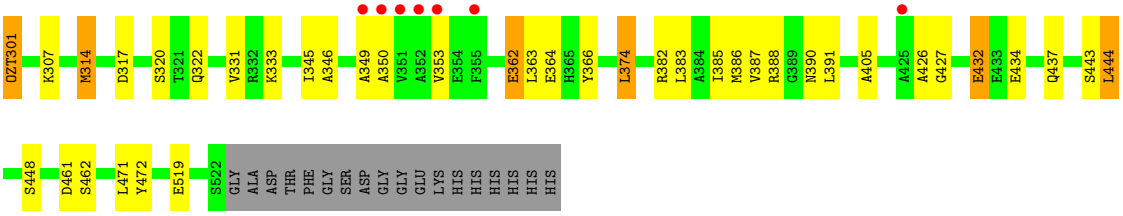
• Molecule 1: Proteasome subunit beta

Chain N:



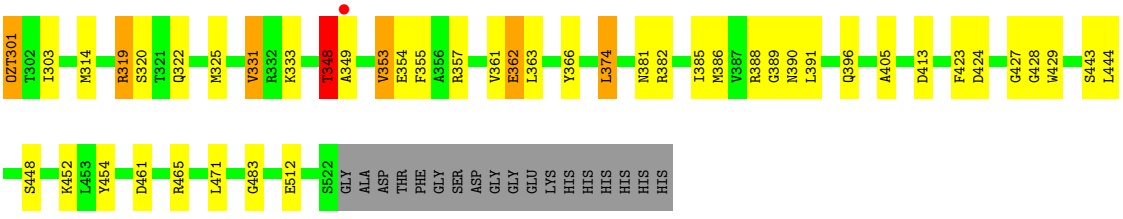
• Molecule 1: Proteasome subunit beta

Chain P:



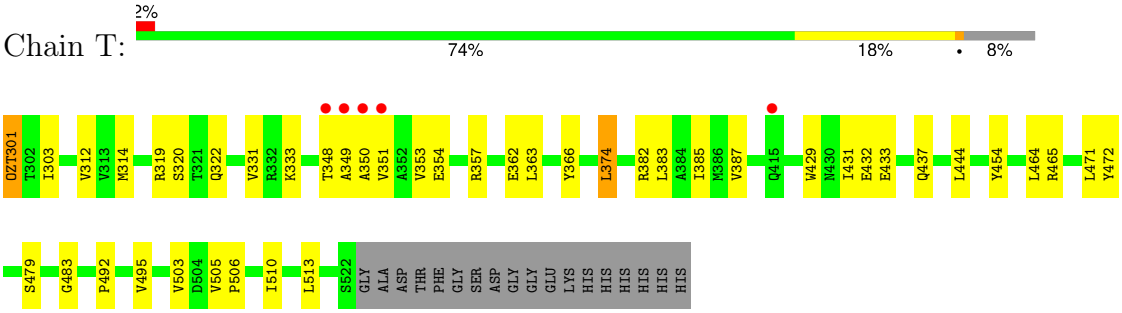
• Molecule 1: Proteasome subunit beta

Chain R:



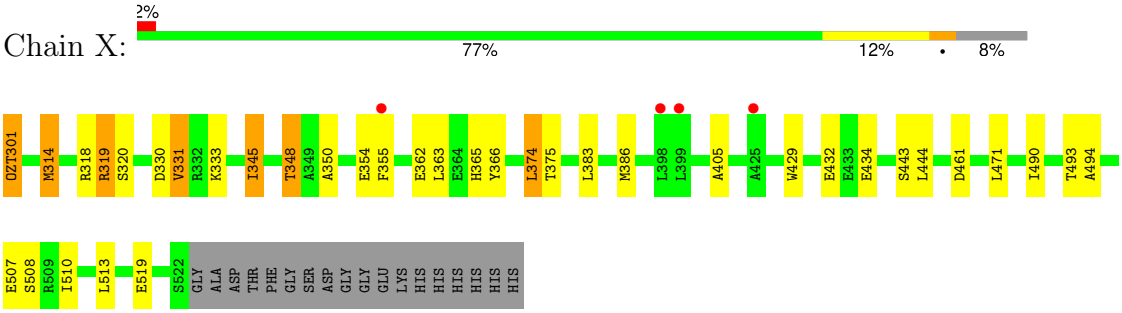
• Molecule 1: Proteasome subunit beta

Chain T:



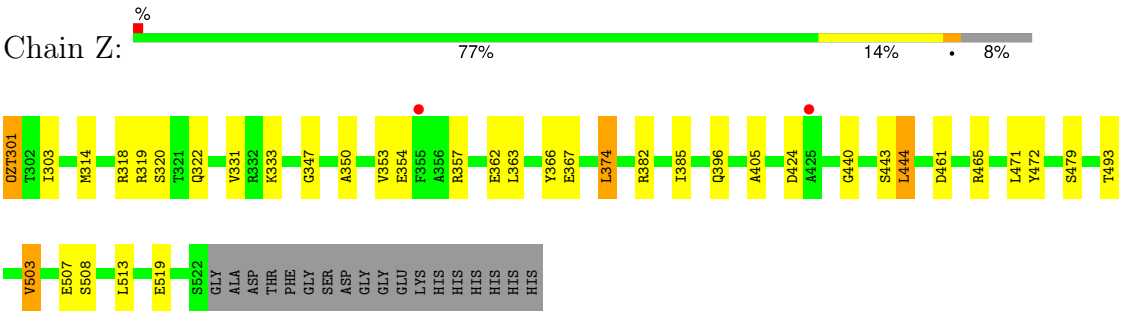
• Molecule 1: Proteasome subunit beta

Chain X:



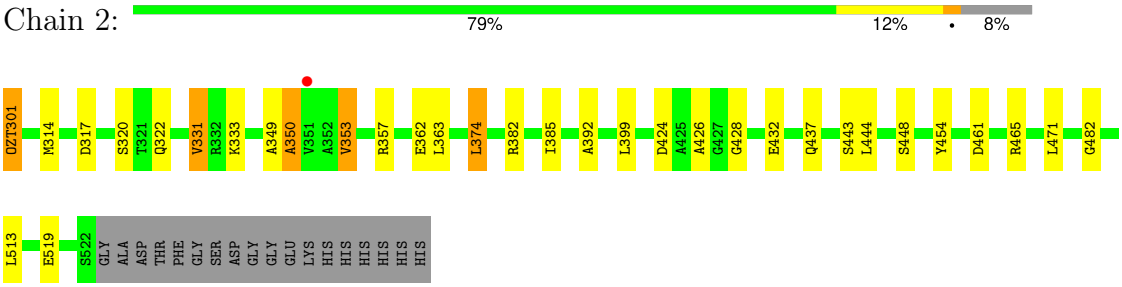
• Molecule 1: Proteasome subunit beta

Chain Z:



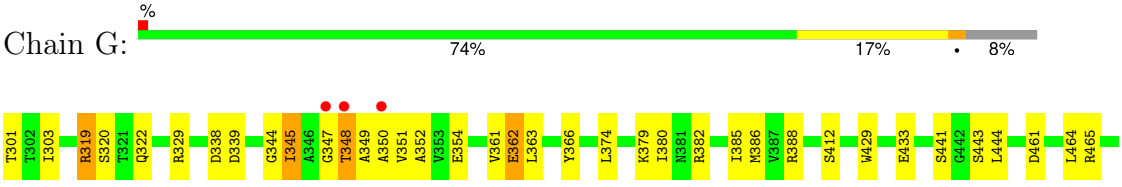
• Molecule 1: Proteasome subunit beta

Chain 2:

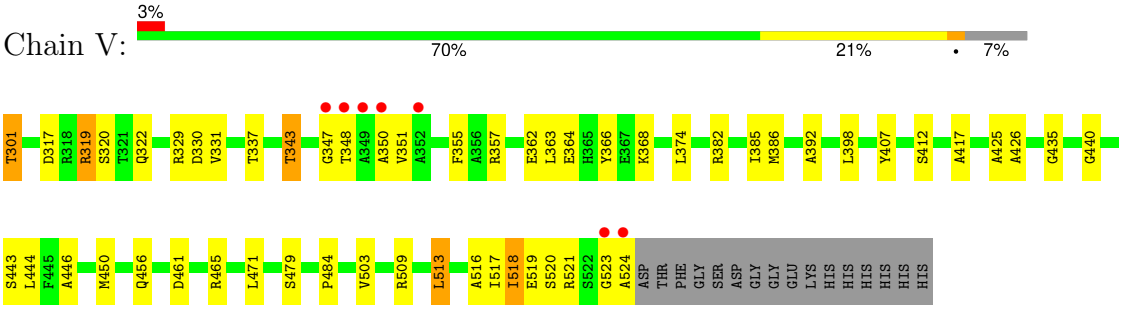


• Molecule 2: Proteasome subunit beta

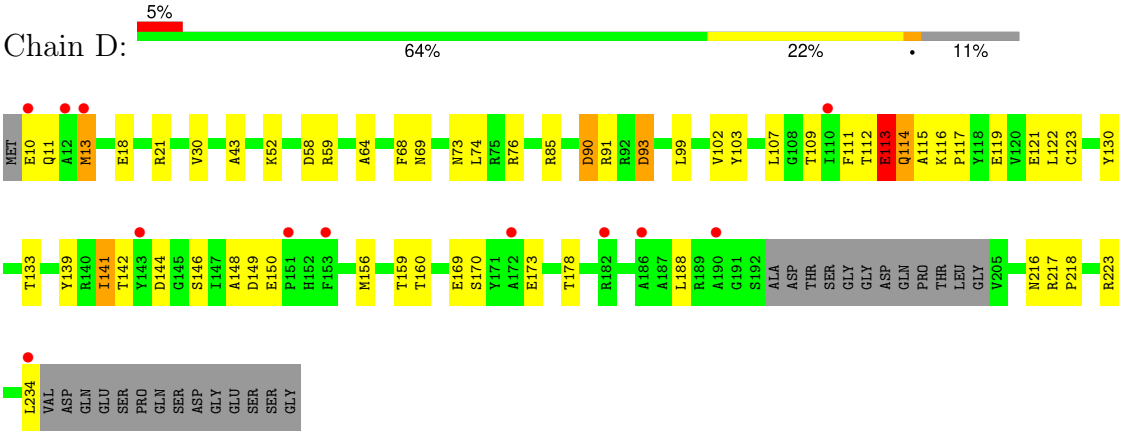
Chain G:



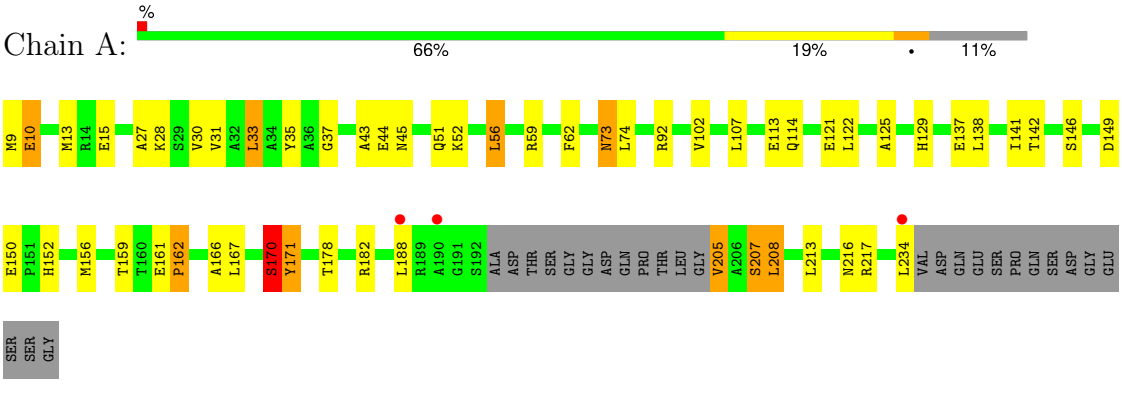
• Molecule 2: Proteasome subunit beta



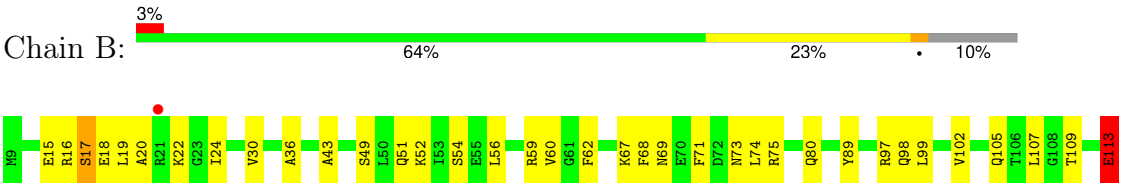
• Molecule 3: Proteasome subunit alpha

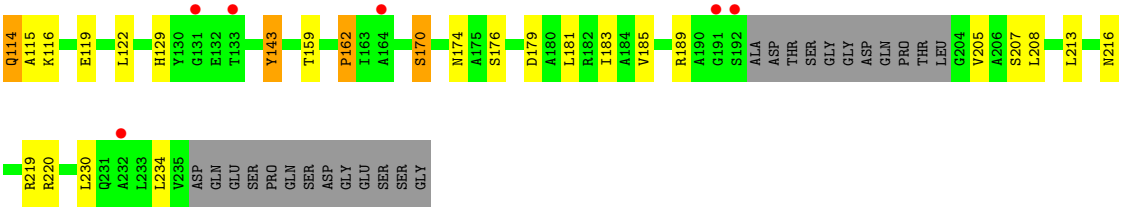


• Molecule 3: Proteasome subunit alpha



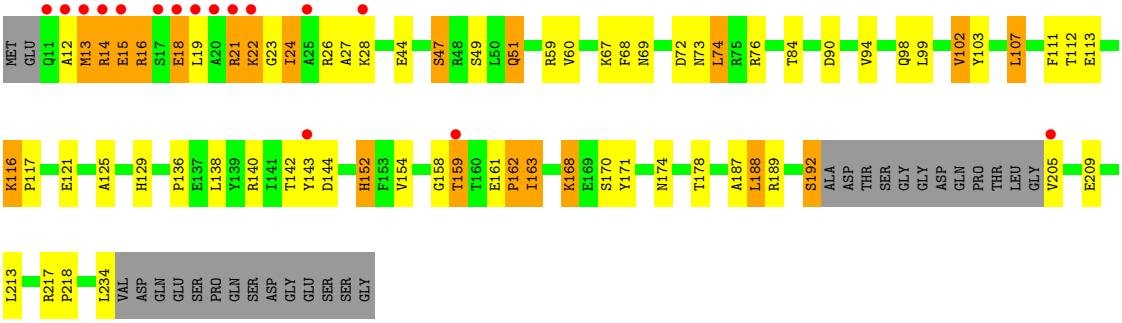
• Molecule 3: Proteasome subunit alpha





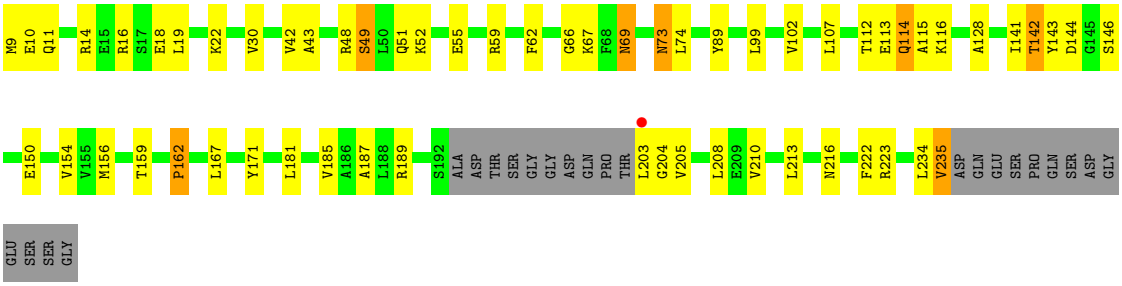
• Molecule 3: Proteasome subunit alpha

Chain F:



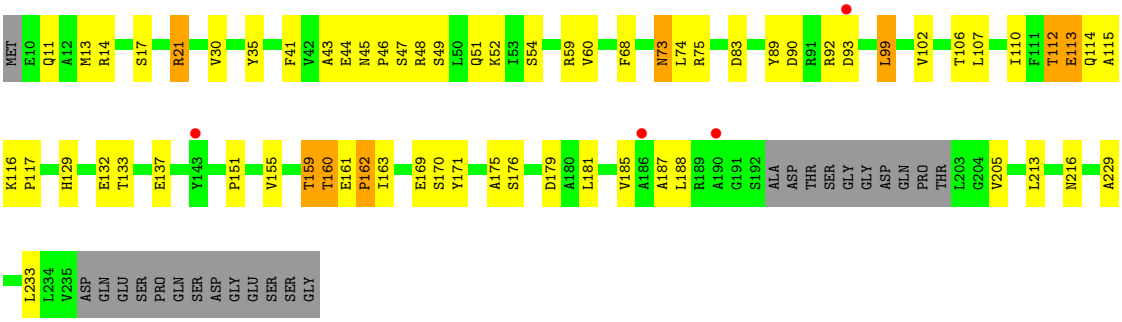
• Molecule 3: Proteasome subunit alpha

Chain I:

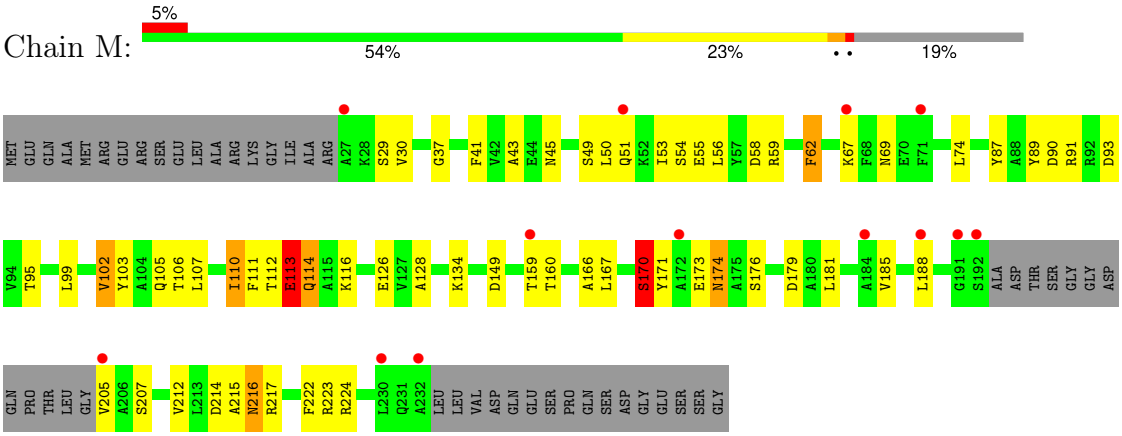


• Molecule 3: Proteasome subunit alpha

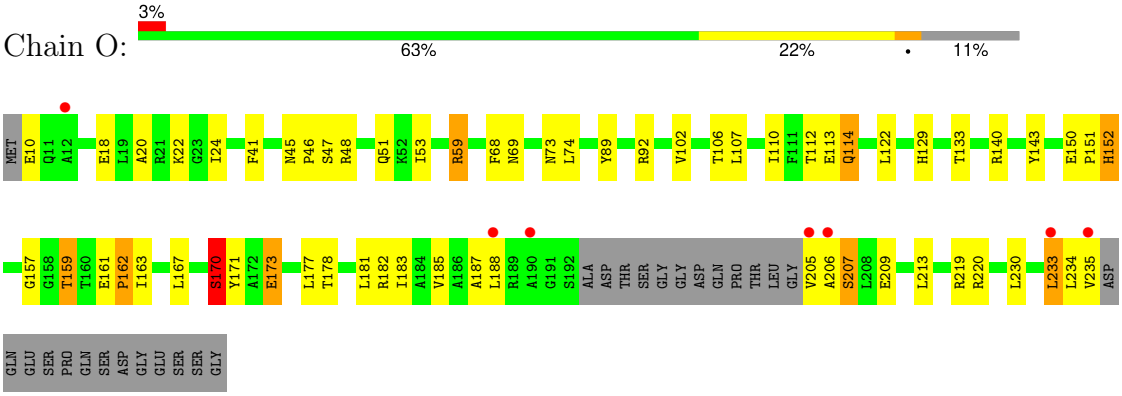
Chain K:



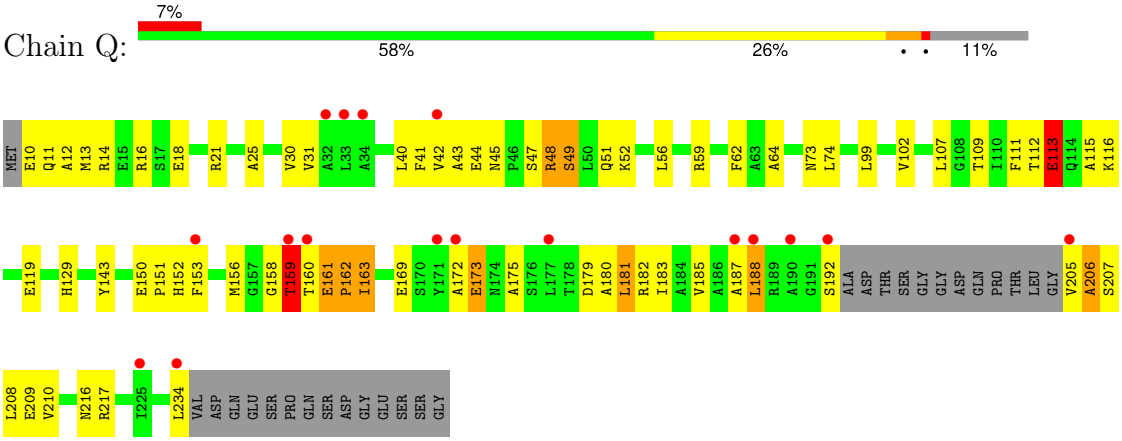
• Molecule 3: Proteasome subunit alpha



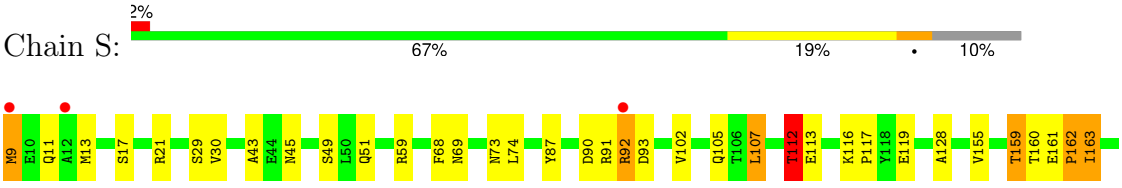
• Molecule 3: Proteasome subunit alpha

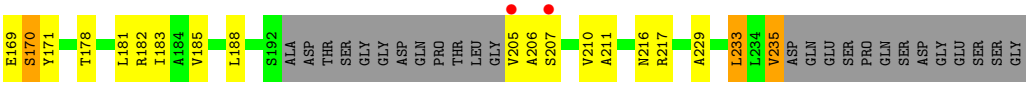


• Molecule 3: Proteasome subunit alpha



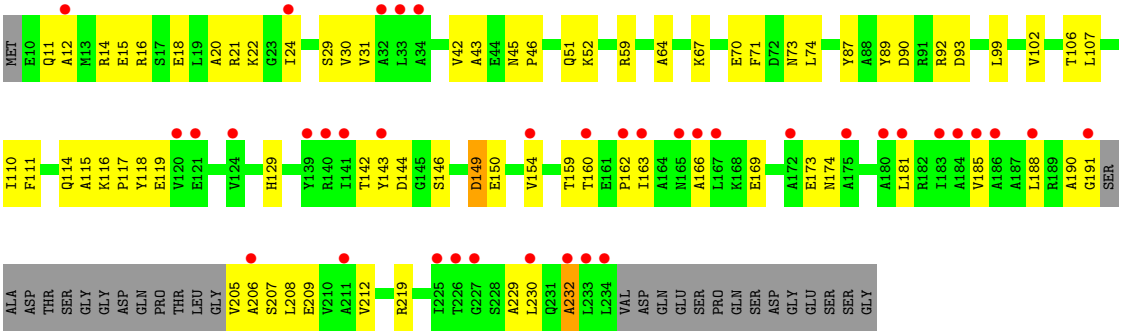
• Molecule 3: Proteasome subunit alpha





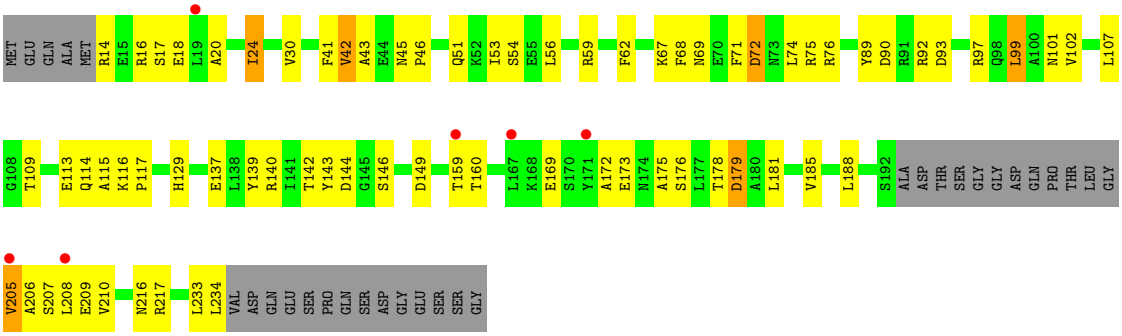
• Molecule 3: Proteasome subunit alpha

Chain U:



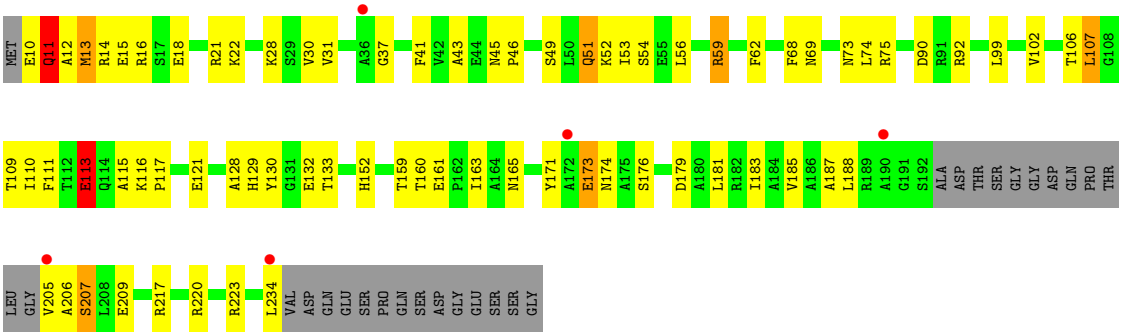
• Molecule 3: Proteasome subunit alpha

Chain W:



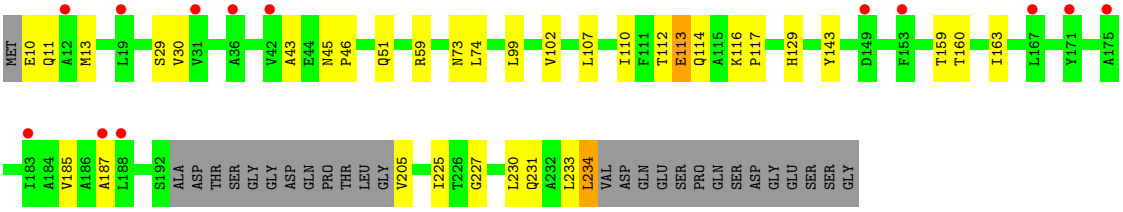
• Molecule 3: Proteasome subunit alpha

Chain Y:



• Molecule 3: Proteasome subunit alpha

Chain 1:


MET E10 Q11 A12 M13 L19 S29 V30 V31 A36 V42 A43 E44 N45 P46 Q51 R59 N73 L74 L99 V102 L107 I110 F111 T112 E113 Q114 A115 K116 P117 H129 Y143 D149 F153 T159 T160 I163 L167 Y171 A175
I183 A184 V185 A186 A187 L188 S192 ALA ASP THR SER GLY GLY ASP GLN PRO THR LEU GLY V205 I225 T226 G227 L230 Q231 A232 L233 L234 VAL ASP GLN GLU SER PRO GLN SER ASP GLY GLU SER SER GLY

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	118.97Å 207.55Å 142.28Å 90.00° 102.42° 90.00°	Depositor
Resolution (Å)	29.87 – 2.60 29.87 – 2.60	Depositor EDS
% Data completeness (in resolution range)	96.5 (29.87-2.60) 96.4 (29.87-2.60)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.90 (at 2.57Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.224 , 0.257 0.219 , 0.250	Depositor DCC
R_{free} test set	9916 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å^2)	38.0	Xtriage
Anisotropy	0.235	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 46.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	46890	wwPDB-VP
Average B, all atoms (Å^2)	53.0	wwPDB-VP

Xtriage'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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.93	2/1655 (0.1%)	1.08	4/2244 (0.2%)
1	C	0.88	0/1655	1.07	2/2244 (0.1%)
1	E	0.91	1/1655 (0.1%)	1.06	5/2244 (0.2%)
1	H	0.93	1/1655 (0.1%)	1.09	6/2244 (0.3%)
1	J	0.89	1/1655 (0.1%)	1.08	5/2244 (0.2%)
1	L	0.92	0/1655	1.09	3/2244 (0.1%)
1	N	1.06	2/1655 (0.1%)	1.10	5/2244 (0.2%)
1	P	1.05	2/1655 (0.1%)	1.08	4/2244 (0.2%)
1	R	0.90	0/1655	1.05	7/2244 (0.3%)
1	T	0.97	3/1655 (0.2%)	1.12	3/2244 (0.1%)
1	X	1.00	2/1655 (0.1%)	1.09	5/2244 (0.2%)
1	Z	0.89	1/1655 (0.1%)	1.11	3/2244 (0.1%)
2	G	0.88	2/1662 (0.1%)	1.12	6/2254 (0.3%)
2	V	1.03	2/1671 (0.1%)	1.05	3/2266 (0.1%)
3	1	0.83	0/1667	1.16	6/2251 (0.3%)
3	A	0.92	0/1675	1.12	11/2261 (0.5%)
3	B	0.94	0/1686	1.12	12/2276 (0.5%)
3	D	0.80	0/1667	1.11	7/2251 (0.3%)
3	F	0.89	1/1658 (0.1%)	1.22	15/2239 (0.7%)
3	I	0.90	1/1694 (0.1%)	1.09	9/2287 (0.4%)
3	K	0.82	1/1686 (0.1%)	1.13	12/2277 (0.5%)
3	M	0.78	0/1513	1.08	7/2048 (0.3%)
3	O	0.86	2/1674 (0.1%)	1.12	13/2261 (0.6%)
3	Q	0.78	1/1667 (0.1%)	1.18	11/2251 (0.5%)
3	S	0.86	1/1682 (0.1%)	1.12	10/2271 (0.4%)
3	U	0.80	0/1661	1.16	6/2243 (0.3%)
3	W	0.76	0/1636	1.02	3/2210 (0.1%)
3	Y	0.80	0/1667	1.07	8/2251 (0.4%)
All	All	0.90	26/46426 (0.1%)	1.10	191/62825 (0.3%)

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	314	MET	SD-CE	-9.35	1.56	1.79
1	P	314	MET	SD-CE	-9.24	1.56	1.79
2	G	361	VAL	C-N	-7.22	1.24	1.33
1	N	314	MET	SD-CE	-7.19	1.61	1.79
1	2	314	MET	SD-CE	-6.82	1.62	1.79
1	X	314	MET	SD-CE	-6.60	1.63	1.79
3	F	159	THR	C-O	6.34	1.31	1.23
1	T	314	MET	SD-CE	-6.29	1.63	1.79
2	G	386	MET	SD-CE	-6.11	1.64	1.79
1	H	314	MET	SD-CE	-5.59	1.65	1.79
2	V	450	MET	SD-CE	-5.49	1.65	1.79
1	Z	503	VAL	CA-CB	5.49	1.62	1.54
3	Q	159	THR	C-O	5.47	1.30	1.23
3	O	159	THR	C-O	5.43	1.30	1.23
1	P	462	SER	CA-C	5.27	1.59	1.52
1	2	353	VAL	CA-CB	5.27	1.61	1.54
3	S	159	THR	CA-C	5.23	1.59	1.53
1	J	314	MET	SD-CE	-5.23	1.66	1.79
3	K	159	THR	C-O	5.20	1.30	1.23
1	X	348	THR	CA-CB	5.11	1.60	1.53
1	T	495	VAL	CA-CB	5.07	1.62	1.54
3	I	66	GLY	C-O	-5.07	1.21	1.24
2	V	446	ALA	CA-CB	-5.06	1.45	1.53
3	O	159	THR	CA-C	5.03	1.59	1.53
1	T	312	VAL	CA-CB	5.03	1.62	1.55
1	N	494	ALA	CA-CB	-5.01	1.45	1.53

All (191) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	49	SER	N-CA-C	10.69	122.93	111.28
3	1	113	GLU	N-CA-C	9.51	121.41	111.14
3	I	49	SER	N-CA-C	9.43	121.64	111.36
3	B	113	GLU	N-CA-C	9.16	122.96	111.69
3	D	173	GLU	N-CA-C	9.12	122.37	111.33
3	Y	11	GLN	N-CA-C	-8.72	101.77	111.28
3	1	11	GLN	N-CA-C	-8.63	102.29	113.17
3	Q	49	SER	N-CA-C	8.62	120.75	111.36
3	Y	113	GLU	N-CA-C	8.49	120.31	111.14
3	A	113	GLU	N-CA-C	8.34	120.45	111.36
3	F	49	SER	N-CA-C	8.28	120.39	111.36
3	K	113	GLU	N-CA-C	8.21	120.31	111.36
3	O	113	GLU	N-CA-C	8.01	120.09	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	I	113	GLU	N-CA-C	8.00	120.08	111.36
3	Q	113	GLU	N-CA-C	7.98	120.06	111.36
3	A	170	SER	N-CA-C	7.87	119.94	111.36
3	M	49	SER	N-CA-C	7.70	119.75	111.36
3	Q	206	ALA	N-CA-C	-7.52	103.08	111.28
3	F	12	ALA	N-CA-C	7.50	119.54	111.36
1	Z	347	GLY	N-CA-C	7.50	122.74	111.42
3	A	10	GLU	N-CA-C	7.46	119.11	110.97
3	Q	173	GLU	N-CA-C	7.40	119.34	111.28
3	M	113	GLU	N-CA-C	7.29	119.31	111.36
3	K	49	SER	N-CA-C	7.28	122.16	113.28
3	M	160	THR	N-CA-C	7.25	119.27	111.36
3	S	160	THR	N-CA-C	7.22	119.15	111.28
3	S	170	SER	N-CA-C	7.14	122.16	113.17
3	1	160	THR	N-CA-C	7.12	119.12	111.36
3	W	160	THR	N-CA-C	7.05	119.04	111.36
3	U	160	THR	N-CA-C	6.99	118.98	111.36
3	K	160	THR	N-CA-C	6.91	118.81	111.28
3	F	170	SER	N-CA-C	6.88	121.76	112.88
3	Q	160	THR	N-CA-C	6.88	118.78	111.28
2	G	348	THR	N-CA-C	-6.83	100.05	110.30
3	I	205	VAL	N-CA-C	6.82	117.57	110.62
1	J	434	GLU	N-CA-C	6.71	120.92	112.87
3	K	51	GLN	N-CA-C	6.70	119.86	109.07
3	1	51	GLN	N-CA-C	6.67	120.69	109.76
3	F	13	MET	N-CA-C	6.66	118.19	111.07
3	O	173	GLU	N-CA-C	6.63	118.50	111.28
3	Y	49	SER	N-CA-C	6.62	118.58	111.36
3	K	114	GLN	N-CA-C	6.59	119.23	110.53
3	U	29	SER	N-CA-C	6.57	120.39	109.95
3	O	152	HIS	N-CA-C	6.56	121.66	112.93
3	S	112	THR	N-CA-C	6.54	118.49	111.36
1	N	413	ASP	CA-C-N	6.47	126.16	119.56
1	N	413	ASP	C-N-CA	6.47	126.16	119.56
3	F	15	GLU	N-CA-C	-6.43	104.19	111.07
3	M	29	SER	N-CA-C	6.42	120.29	109.76
3	A	51	GLN	N-CA-C	6.40	120.25	109.76
3	S	171	TYR	N-CA-C	6.38	119.52	109.96
3	K	68	PHE	N-CA-C	6.36	118.78	111.02
2	V	518	ILE	N-CA-C	6.36	116.50	110.53
3	K	162	PRO	CA-C-N	-6.34	111.77	120.46
3	K	162	PRO	C-N-CA	-6.34	111.77	120.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	X	354	GLU	N-CA-C	6.30	118.14	111.28
3	Q	47	SER	N-CA-C	6.30	119.41	109.96
3	D	13	MET	N-CA-C	6.28	120.04	112.38
3	F	213	LEU	N-CA-C	-6.24	95.33	107.62
3	O	162	PRO	CA-C-N	-6.23	111.93	120.46
3	O	162	PRO	C-N-CA	-6.23	111.93	120.46
3	F	51	GLN	N-CA-C	6.19	119.04	109.07
3	U	232	ALA	N-CA-C	6.17	119.90	112.38
3	D	113	GLU	N-CA-C	6.12	118.03	111.36
3	Y	160	THR	N-CA-C	6.05	117.96	111.36
3	W	68	PHE	N-CA-C	6.04	118.38	111.02
1	H	351	VAL	N-CA-C	-6.03	105.86	112.80
3	F	159	THR	CA-C-O	6.00	128.49	121.11
1	H	472	TYR	N-CA-C	-5.99	104.67	111.14
1	Z	443	SER	N-CA-C	5.98	118.57	111.33
3	O	114	GLN	N-CA-C	5.97	118.41	110.53
1	E	453	LEU	N-CA-C	5.95	120.54	113.28
1	H	353	VAL	N-CA-C	5.94	116.68	110.62
3	I	162	PRO	CA-C-N	-5.93	112.33	120.46
3	I	162	PRO	C-N-CA	-5.93	112.33	120.46
3	F	162	PRO	CA-C-N	-5.92	112.35	120.46
3	F	162	PRO	C-N-CA	-5.92	112.35	120.46
1	R	443	SER	N-CA-C	5.90	118.49	111.71
1	N	331	VAL	N-CA-C	5.89	116.88	108.93
1	R	331	VAL	N-CA-C	5.87	116.99	109.30
3	S	68	PHE	N-CA-C	5.84	118.15	111.02
3	F	47	SER	N-CA-C	5.84	119.04	109.76
3	F	22	LYS	N-CA-C	-5.81	104.95	111.28
3	Y	206	ALA	N-CA-C	-5.80	106.05	113.01
3	U	173	GLU	N-CA-C	5.79	117.39	111.14
3	B	51	GLN	N-CA-C	5.77	118.35	109.07
3	I	114	GLN	N-CA-C	5.76	118.13	110.53
3	K	60	VAL	N-CA-C	5.76	116.23	108.17
3	I	143	TYR	N-CA-C	5.73	118.30	111.71
1	E	331	VAL	N-CA-C	5.71	116.44	109.30
3	K	14	ARG	N-CA-C	-5.71	106.97	114.04
3	Q	162	PRO	CA-C-N	-5.69	112.66	120.46
3	Q	162	PRO	C-N-CA	-5.69	112.66	120.46
1	J	331	VAL	N-CA-C	5.69	116.41	109.30
3	B	143	TYR	N-CA-C	5.69	119.03	111.75
3	B	162	PRO	CA-C-N	-5.69	112.67	120.46
3	B	162	PRO	C-N-CA	-5.69	112.67	120.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	I	51	GLN	N-CA-C	5.68	118.65	109.40
3	Q	152	HIS	N-CA-C	5.67	121.07	114.04
3	A	122	LEU	N-CA-C	5.65	118.77	109.72
1	C	413	ASP	CA-C-N	5.64	125.31	119.56
1	C	413	ASP	C-N-CA	5.64	125.31	119.56
1	N	454	TYR	N-CA-C	5.61	118.94	111.75
1	E	413	ASP	CA-C-N	5.60	125.27	119.56
1	E	413	ASP	C-N-CA	5.60	125.27	119.56
1	R	319	ARG	N-CA-C	5.59	118.75	110.48
1	T	431	ILE	N-CA-C	-5.58	101.52	108.89
1	X	443	SER	N-CA-C	5.54	117.32	111.28
3	1	29	SER	N-CA-C	5.54	118.67	110.48
2	G	349	ALA	CB-CA-C	-5.51	110.20	116.54
2	G	319	ARG	N-CA-C	5.51	118.63	110.48
3	M	114	GLN	N-CA-C	5.50	118.26	110.50
3	S	51	GLN	N-CA-C	5.49	117.92	109.07
2	G	443	SER	N-CA-C	5.48	117.25	111.28
1	P	432	GLU	N-CA-C	5.45	118.13	109.96
3	B	114	GLN	N-CA-C	5.43	117.88	110.55
1	P	345	ILE	N-CA-C	5.42	116.39	108.53
1	X	345	ILE	O-C-N	-5.41	117.46	123.20
3	W	72	ASP	N-CA-C	-5.40	105.43	112.23
3	S	162	PRO	CA-C-N	-5.39	113.08	120.46
3	S	162	PRO	C-N-CA	-5.39	113.08	120.46
3	S	49	SER	N-CA-C	5.38	119.95	113.17
3	I	213	LEU	N-CA-C	-5.38	96.54	107.41
3	A	171	TYR	N-CA-C	5.37	118.02	109.96
1	X	319	ARG	N-CA-C	5.37	118.06	110.50
3	O	207	SER	N-CA-C	-5.36	106.11	113.56
1	L	413	ASP	CA-C-N	5.36	125.03	119.56
1	L	413	ASP	C-N-CA	5.36	125.03	119.56
1	J	454	TYR	N-CA-C	5.35	117.86	111.71
1	R	413	ASP	CA-C-N	5.35	125.02	119.56
1	R	413	ASP	C-N-CA	5.35	125.02	119.56
3	Y	68	PHE	N-CA-C	5.35	117.55	111.02
3	B	213	LEU	N-CA-C	-5.34	96.61	107.41
1	N	346	ALA	N-CA-C	5.34	118.02	107.98
3	D	160	THR	N-CA-C	5.33	116.89	111.14
2	V	319	ARG	N-CA-C	5.30	118.32	110.48
1	2	454	TYR	N-CA-C	5.30	117.80	111.71
3	F	152	HIS	N-CA-C	5.30	119.98	112.93
3	D	170	SER	N-CA-C	5.29	119.73	113.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	Y	51	GLN	N-CA-C	5.29	118.02	109.40
3	F	60	VAL	N-CA-C	5.28	115.56	108.17
3	O	122	LEU	N-CA-C	5.27	118.33	109.95
3	B	122	LEU	N-CA-C	5.26	118.32	109.95
3	B	170	SER	N-CA-C	5.26	119.00	112.59
1	R	454	TYR	N-CA-C	5.25	117.75	111.71
1	2	443	SER	N-CA-C	5.24	116.99	111.28
3	F	68	PHE	N-CA-C	5.23	117.40	111.02
1	P	472	TYR	N-CA-C	-5.23	105.49	111.14
1	H	331	VAL	N-CA-C	5.22	115.83	109.30
3	B	208	LEU	N-CA-C	5.22	117.62	109.52
1	T	454	TYR	N-CA-C	5.22	117.71	111.71
1	E	443	SER	N-CA-C	5.21	116.96	111.28
3	K	205	VAL	N-CA-C	5.20	115.81	110.36
2	V	443	SER	N-CA-C	5.19	116.94	111.28
3	A	213	LEU	N-CA-C	-5.19	96.92	107.41
3	A	162	PRO	CA-C-N	-5.19	113.35	120.46
3	A	162	PRO	C-N-CA	-5.19	113.35	120.46
3	1	143	TYR	N-CA-C	5.17	118.36	111.75
3	U	143	TYR	N-CA-C	5.16	118.36	111.75
1	H	454	TYR	N-CA-C	5.16	117.65	111.71
1	2	331	VAL	N-CA-C	5.16	115.75	109.30
3	K	170	SER	N-CA-C	5.16	119.57	113.28
1	R	348	THR	N-CA-C	5.15	117.33	110.53
3	D	68	PHE	N-CA-C	5.15	117.30	111.02
2	G	339	ASP	N-CA-C	5.14	117.62	111.71
3	Q	169	GLU	N-CA-C	5.12	116.94	111.36
2	G	380	ILE	CB-CA-C	-5.11	105.43	111.97
3	Y	173	GLU	N-CA-C	5.11	118.61	112.38
3	O	171	TYR	N-CA-C	5.10	117.70	110.10
3	O	143	TYR	N-CA-C	5.10	118.28	111.75
3	Q	143	TYR	N-CA-C	5.10	118.27	111.75
1	T	472	TYR	N-CA-C	-5.09	105.64	111.14
3	O	68	PHE	N-CA-C	5.09	117.23	111.02
1	J	413	ASP	CA-C-N	5.08	124.74	119.56
1	J	413	ASP	C-N-CA	5.08	124.74	119.56
3	M	170	SER	N-CA-C	5.08	119.48	113.28
3	A	56	LEU	N-CA-C	-5.07	106.19	112.93
1	L	331	VAL	N-CA-C	5.07	115.53	108.84
3	S	29	SER	N-CA-C	5.07	118.38	110.32
1	X	331	VAL	N-CA-C	5.06	115.63	109.30
1	P	443	SER	N-CA-C	5.05	117.44	111.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	H	443	SER	N-CA-C	5.05	117.52	111.71
3	O	213	LEU	N-CA-C	-5.05	97.67	107.62
3	D	122	LEU	N-CA-C	5.05	117.97	109.95
3	B	60	VAL	N-CA-C	5.04	115.22	108.17
3	U	51	GLN	N-CA-C	5.03	117.69	109.59
3	M	110	ILE	CB-CA-C	-5.02	105.37	112.14
1	2	350	ALA	N-CA-C	5.02	116.56	111.14
3	A	208	LEU	N-CA-C	5.01	117.32	110.55
1	Z	472	TYR	N-CA-C	-5.01	105.90	111.36
3	O	170	SER	N-CA-C	5.00	119.38	113.28

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	32	0
1	C	1640	0	1630	42	0
1	E	1640	0	1630	31	0
1	H	1640	0	1630	31	0
1	J	1640	0	1630	23	0
1	L	1640	0	1630	39	0
1	N	1640	0	1630	38	0
1	P	1640	0	1630	37	0
1	R	1640	0	1630	39	0
1	T	1640	0	1630	40	0
1	X	1640	0	1630	33	0
1	Z	1640	0	1630	26	0
2	G	1638	0	1630	31	0
2	V	1647	0	1638	69	0
3	1	1643	0	1641	29	0
3	A	1651	0	1650	52	0
3	B	1662	0	1662	38	0
3	D	1643	0	1641	44	0
3	F	1634	0	1635	80	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	I	1670	0	1673	56	0
3	K	1662	0	1664	54	0
3	M	1489	0	1474	58	0
3	O	1650	0	1650	66	0
3	Q	1643	0	1641	78	0
3	S	1658	0	1659	57	0
3	U	1637	0	1636	76	0
3	W	1612	0	1613	44	0
3	Y	1643	0	1641	57	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	3	0
4	D	18	0	0	8	0
4	E	38	0	0	7	0
4	F	33	0	0	1	0
4	G	41	0	0	3	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
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	1191	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 (1191) 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:Q:181:LEU:C	3:Q:181:LEU:HD12	1.55	1.29
3:U:163:ILE:CG1	3:U:191:GLY:HA3	1.65	1.27
1:C:349:ALA:O	1:C:353:VAL:HG22	1.38	1.24
3:Q:18:GLU:CD	3:Q:21:ARG:HH12	1.45	1.24
3:Q:180:ALA:HA	3:Q:183:ILE:HD12	1.22	1.21
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
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
3:Q:205:VAL:HG13	3:Q:206:ALA:H	1.12	1.06
3:Y:13:MET:HE3	3:Y:13:MET:HA	1.34	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:Q:181:LEU:C	3:Q:181:LEU:CD1	2.31	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
1:2:301:OZT:C7	1:2:333:LYS:NZ	2.24	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:2:301:OZT:H17	1:2:333:LYS:HZ1	1.19	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:N:359:TYR:HA	1:N:386:MET:HE1	1.44	0.97
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: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:Q:205:VAL:HG13	3:Q:206:ALA:N	1.67	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
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
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
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
1:X:301:OZT:H17	1:X:333:LYS:HZ1	1.33	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:A:137:GLU:CD	3:O:48:ARG:HH21	1.80	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:K:44:GLU:HG2	4:K:984:HOH:O	1.72	0.88
3:Q:18:GLU:CD	3:Q:21:ARG:NH1	2.31	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:I:19:LEU:CD2	3:S:9:MET:HE1	2.04	0.87
3:F:168:LYS:NZ	3:F:168:LYS:CB	2.30	0.87
3:1:231:GLN:C	3:1:234:LEU:HD12	1.99	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
1:2:301:OZT:C7	1:2:333:LYS:HZ3	1.85	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:F:21:ARG:HD2	3:F:21:ARG:C	2.01	0.85
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
1:N:359:TYR:CA	1:N:386:MET:HE1	2.06	0.84
1:H:391:LEU:HD12	1:H:391:LEU:C	2.01	0.84
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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:517:ILE:O	2:V:521:ARG:HG3	1.79	0.82
1:X:301:OZT:H17	1:X:333:LYS:HZ3	1.43	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
1:P:301:OZT:C7	1:P:333:LYS:NZ	2.43	0.81
1:J:301:OZT:H17	1:J:333:LYS:HZ3	1.44	0.81
1:J:301:OZT:H17	1:J:333:LYS:NZ	1.95	0.81
3:U:16:ARG:HH12	3:U:111:PHE:C	1.87	0.81
1:P:301:OZT:H27	1:P:333:LYS:HZ1	1.46	0.80
1:2:301:OZT:H17	1:2:333:LYS:HZ3	0.99	0.80
1:X:301:OZT:C7	1:X:333:LYS:HZ1	1.94	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
1:H:301:OZT:H17	1:H:333:LYS:HZ3	1.42	0.80
3:I:142:THR:CG2	3:I:144:ASP:OD1	2.30	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
3:1:231:GLN:C	3:1:234:LEU:CD1	2.55	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
3:Q:179:ASP:O	3:Q:183:ILE:CG1	2.30	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:L:301:OZT:H17	1:L:333:LYS:HZ3	1.48	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
3:S:161:GLU:CD	3:S:161:GLU:H	1.92	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
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:I:19:LEU:HD22	3:S:9:MET:HE1	1.67	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: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:U:149:ASP:OD1	3:U:149:ASP:C	2.30	0.74
1:C:354:GLU:OE2	1:C:354:GLU:C	2.30	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
2:V:523:GLY:O	2:V:524:ALA:C	2.32	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
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:E:301:OZT:H2	4:E:876:HOH:O	1.89	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:33:LEU:N	3:A:33:LEU:HD23	2.05	0.72
3:W:92:ARG:HH11	3:W:92:ARG:HB3	1.54	0.72
2:V:456:GLN:CD	2:V:465:ARG:HH22	1.97	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
2:G:344:GLY:C	2:G:345:ILE:HD12	2.14	0.71
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
1:X:301:OZT:C7	1:X:333:LYS:HZ3	2.00	0.71
3:W:90:ASP:HB3	3:W:93:ASP:OD2	1.91	0.71
3:F:16:ARG:NH1	3:F:16:ARG:C	2.49	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
1:J:355:PHE:CE2	1:J:386:MET:HE2	2.27	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:F:152:HIS:HB3	3:F:171:TYR:CE2	2.28	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
1:2:301:OZT:C7	1:2:333:LYS:HZ1	1.95	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
3:A:150:GLU:HA	3:A:150:GLU:OE2	1.92	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
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
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:F:140:ARG:HD2	3:F:154:VAL:HG13	1.76	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:117:PRO:HG2	4:D:930:HOH:O	1.95	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
3:U:116:LYS:HZ1	3:U:119:GLU:HG3	1.61	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: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:K:161:GLU:H	3:K:161:GLU:CD	2.04	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:1:230:LEU:C	3:1:234:LEU:HD11	2.23	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
1:N:301:OZT:H17	1:N:333:LYS:HZ3	1.60	0.63
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
2:V:456:GLN:CD	2:V:465:ARG:NH2	2.56	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:I:189:ARG:HD3	3:I:189:ARG:C	2.23	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
1:P:350:ALA:CB	2:V:426:ALA:HB3	2.29	0.62
2:V:350:ALA:CB	1:2:424:ASP:OD2	2.47	0.62
3:B:17:SER:HG	3:B:143:TYR:HE1	1.47	0.62
3:S:59:ARG:NH1	3:S:128:ALA:O	2.32	0.62
3:A:149:ASP:CG	3:O:48:ARG:NH1	2.57	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
3:O:205:VAL:HG13	3:O:230:LEU:HD23	1.79	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:N:362:GLU:OE2	1:N:382:ARG:NH1	2.30	0.62
1:R:388:ARG:C	1:R:390:ASN:H	2.07	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
3:A:52:LYS:NZ	4:A:651:HOH:O	2.31	0.62
1:C:452:LYS:NZ	4:C:234:HOH:O	2.33	0.61
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:L:355:PHE:CE1	1:L:386:MET:HE2	2.36	0.61
1:T:348:THR:O	1:T:351:VAL:HG12	2.01	0.61
3:S:205:VAL:C	3:S:207:SER:H	2.09	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:M:62:PHE:C	3:M:62:PHE:CD2	2.78	0.61
3:Q:18:GLU:OE1	3:Q:21:ARG:NH1	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
1:X:355:PHE:HZ	1:X:383:LEU:HD11	1.66	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:Y:52:LYS:NZ	4:Y:415:HOH:O	2.30	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
3:S:112:THR:HG22	3:S:113:GLU:CG	2.26	0.58
3:S:161:GLU:CD	3:S:161:GLU:N	2.60	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
2:G:301:THR:N	2:G:441:SER:HG	2.02	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:Q:181:LEU:HD12	3:Q:182:ARG:N	2.16	0.58
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:I:116:LYS:HB2	3:S:13:MET:HE3	1.86	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:K:161:GLU:CD	3:K:161:GLU:N	2.62	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:1:163:ILE:HG23	3:1:187:ALA:HB1	1.85	0.58
1:L:390:ASN:CG	1:L:390:ASN:O	2.46	0.58
3:I:16:ARG:NH2	3:I:114:GLN:O	2.36	0.58
3:Q:18:GLU:OE2	3:Q:21:ARG:NH1	2.30	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: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:B:67:LYS:HZ2	3:B:69:ASN:HD21	1.51	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
3:Q:172:ALA:CB	3:Q:175:ALA:HB2	2.34	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
1:E:348:THR:HB	1:E:351:VAL:HG23	1.87	0.56
1:P:301:OZT:H17	1:P:333:LYS:NZ	2.20	0.56
1:R:325:MET:HE1	1:Z:444:LEU:HD21	1.87	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
3:M:45:ASN:C	3:M:45:ASN:OD1	2.47	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:Q:13:MET:HE1	3:Q:111:PHE:HE2	1.71	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:354:GLU:OE2	1:C:355:PHE:CA	2.53	0.56
2:G:347:GLY:O	2:G:348:THR:C	2.47	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
3:F:21:ARG:C	3:F:21:ARG:CD	2.68	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:U:16:ARG:NH1	3:U:111:PHE:C	2.61	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:N:432:GLU:CD	1:N:437:GLN:HE21	2.15	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
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: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:E:368:LYS:NZ	4:E:849:HOH:O	2.39	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
3:W:17:SER:HG	3:W:143:TYR:HH	1.56	0.53
3:W:17:SER:OG	3:W:143:TYR:OH	2.27	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:14:ARG:HG3	4:Q:982:HOH:O	2.09	0.53
2:G:350:ALA:O	2:G:351:VAL:C	2.50	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:355:PHE:CE2	1:C:386:MET:HE2	2.44	0.52
3:Y:163:ILE:HG23	3:Y:187:ALA:C	2.34	0.52
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
3:Y:45:ASN:C	3:Y:45:ASN:OD1	2.51	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:I:19:LEU:HD23	3:S:9:MET:HE1	1.89	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:F:51:GLN:CG	3:F:209:GLU:OE2	2.49	0.52
3:S:182:ARG:HH21	3:S:235:VAL:C	2.18	0.52
3:U:116:LYS:NZ	3:U:119:GLU:OE1	2.42	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
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
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: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
1:L:301:OZT:H17	1:L:333:LYS:HZ1	1.74	0.51
3:D:117:PRO:HG3	4:D:930:HOH:O	2.05	0.51
4:B:737:HOH:O	3:I:9:MET:HE3	2.10	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
3:Y:12:ALA:C	3:Y:14:ARG:N	2.67	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
1:L:441:SER:OG	1:L:478:ASP:OD2	2.21	0.51
2:V:347:GLY:O	2:V:348:THR:C	2.51	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:R:388:ARG:C	1:R:390:ASN:N	2.68	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: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: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
1:L:355:PHE:CZ	1:L:386:MET:HE2	2.47	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: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
3:Q:207:SER:C	3:Q:208:LEU:HD23	2.37	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:S:45:ASN:OD1	3:S:45:ASN:C	2.56	0.49
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
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:L:391:LEU:HD12	1:L:391:LEU:C	2.32	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:W:71:PHE:CD1	3:W:71:PHE:C	2.91	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:A:45:ASN:C	3:A:207:SER:O	2.56	0.49
3:M:166:ALA:O	3:M:170:SER:OG	2.20	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:I:19:LEU:CD2	3:S:9:MET:CE	2.81	0.48
3:K:159:THR:O	3:K:163:ILE:HG13	2.12	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
3:S:205:VAL:C	3:S:207:SER:N	2.69	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:K:99:LEU:C	3:K:102:VAL:HG12	2.39	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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
2:G:350:ALA:C	2:G:352:ALA:N	2.65	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:E:301:OZT:H17	1:E:333:LYS:HZ1	1.78	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
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
2:G:354:GLU:CD	1:N:388:ARG:NH2	2.72	0.47
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
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:Y:129:HIS:O	3:Y:130:TYR:C	2.57	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:Z:314:MET:HE3	1:Z:405:ALA:HB2	1.96	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:Y:13:MET:HE3	3:Y:13:MET:CA	2.24	0.47
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:J:314:MET:HE3	1:J:405:ALA:HB2	1.97	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
1:E:314:MET:HE3	1:E:405:ALA:HB2	1.97	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:28:LYS:HZ3	3:Y:46:PRO:CD	2.27	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
3:U:111:PHE:CD2	3:U:111:PHE:C	2.92	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:170:SER:HB2	3:O:183:ILE:HG23	1.95	0.46
1:P:386:MET:HE2	1:P:386:MET:HB3	1.73	0.46
1:X:355:PHE:HZ	1:X:383:LEU:CD1	2.24	0.46
1:2:432:GLU:CD	1:2:437:GLN:HE21	2.23	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:C:354:GLU:C	1:C:354:GLU:CD	2.83	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
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:Q:156:MET:HE3	3:Q:156:MET:HB2	1.73	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: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:390:ASN:CG	1:R:390:ASN:O	2.59	0.46
1:T:348:THR:C	1:T:351:VAL:HG12	2.40	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:Q:153:PHE:CD1	3:Q:153:PHE:C	2.94	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
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: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:N:424:ASP:OD1	1:N:424:ASP:C	2.59	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
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
3:M:214:ASP:OD1	3:M:214:ASP:C	2.60	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:K:47:SER:OG	3:M:149:ASP:OD2	2.33	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:N:359:TYR:HA	1:N:386:MET:CE	2.29	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:R:366:TYR:CD2	1:R:374:LEU:HD13	2.53	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: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:H:301:OZT:H17	1:H:333:LYS:HZ1	1.78	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:I:234:LEU:C	3:I:234:LEU:HD12	2.42	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:L:314:MET:HE3	1:L:405:ALA:HB2	1.99	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
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
1:X:355:PHE:CE1	1:X:386:MET:HE2	2.53	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
3:I:62:PHE:CD2	3:I:62:PHE:C	2.95	0.44
3:W:67:LYS:HZ2	3:W:69:ASN:HD21	1.66	0.44
1:N:359:TYR:CB	1:N:386:MET:HE1	2.48	0.44
1:P:307:LYS:HD3	4:P:541:HOH:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:465:ARG:HG3	1:T:513:LEU:HD22	1.99	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:J:358:LEU:HD23	1:J:386:MET:HE3	1.99	0.44
1:P:314:MET:HE3	1:P:405:ALA:HB2	2.00	0.44
1:R:349:ALA:O	1:R:353:VAL:HG23	2.18	0.44
2:V:330:ASP:OD1	2:V:330:ASP:N	2.50	0.44
3:K:171:TYR:C	3:K:171:TYR:CD2	2.95	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
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: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
3:U:144:ASP:CG	3:U:146:SER:HG	2.25	0.43
1:P:390:ASN:CG	1:P:390:ASN:O	2.61	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
2:G:350:ALA:C	2:G:352:ALA:H	2.26	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:355:PHE:CZ	2:V:386:MET:HE2	2.53	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: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:U:229:ALA:HB2	4:U:411:HOH:O	2.19	0.43
3:Y:10:GLU:CD	3:Y:10:GLU:C	2.86	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: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
3:S:59:ARG:NH2	3:S:217:ARG:O	2.50	0.43
3:S:91:ARG:C	3:S:93:ASP:H	2.27	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
1:2:317:ASP:CG	1:2:333:LYS:HZ2	2.26	0.43
3:I:10:GLU:HB3	3:I:14:ARG:HH21	1.83	0.43
3:U:116:LYS:NZ	3:U:117:PRO:O	2.51	0.43
1:L:333:LYS:O	1:L:344:GLY:HA2	2.19	0.43
1:R:314:MET:HE3	1:R:405:ALA:HB2	2.01	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:N:423:PHE:CD2	1:N:423:PHE:N	2.87	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:M:58:ASP:CG	3:M:91:ARG:HH21	2.25	0.42
3:U:90:ASP:O	3:U:93:ASP:HB2	2.19	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
1:T:432:GLU:CD	1:T:437:GLN:HE21	2.27	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
3:D:148:ALA:C	4:D:603:HOH:O	2.62	0.42
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:M:176:SER:HB3	3:M:179:ASP:CG	2.45	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
3:I:9:MET:HE3	3:I:9:MET:HB2	1.97	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:301:OZT:H17	1:E:333:LYS:HZ3	1.84	0.42
2:G:465:ARG:HG3	2:G:513:LEU:HD22	2.02	0.42
1:X:314:MET:HE3	1:X:405:ALA:HB2	2.01	0.42
3:F:67:LYS:HG2	3:F:69:ASN:HD21	1.85	0.42
3:W:109:THR:O	3:W:113:GLU:HB2	2.20	0.42
1:C:314:MET:HE3	1:C:405:ALA:HB2	2.02	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
3:B:176:SER:HB3	3:B:179:ASP:OD2	2.20	0.41
3:F:159:THR:HG22	3:F:159:THR:O	2.20	0.41
3:I:156:MET:HE3	3:I:156:MET:HB2	1.97	0.41
3:Q:181:LEU:CD1	3:Q:185:VAL:HG23	2.50	0.41
3:W:45:ASN:HA	3:W:46:PRO:HD2	1.97	0.41
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:10:GLU:C	3:Q:12:ALA:N	2.78	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:H:314:MET:HE3	1:H:405:ALA:HB2	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:U:71:PHE:CD1	3:U:71:PHE:C	2.98	0.41
3:U:116:LYS:HZ1	3:U:119:GLU:CG	2.31	0.41
3:Y:69:ASN:HD22	3:Y:69:ASN:H	1.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:R:355:PHE:CE1	1:R:386:MET:HE2	2.55	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:O:206:ALA:O	3:O:207:SER:OG	2.30	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
1:H:432:GLU:CD	1:H:437:GLN:HE21	2.29	0.41
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
3:A:73:ASN:HD21	3:B:105:GLN:HG3	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:149:ASP:OD1	3:A:149:ASP:C	2.64	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
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:S:116:LYS:HB2	3:1:112:THR:HG23	2.03	0.40
3:U:116:LYS:CE	3:U:119:GLU:OE1	2.69	0.40
3:W:181:LEU:O	3:W:185:VAL:HG23	2.21	0.40
3:Y:205:VAL:C	3:Y:207:SER:N	2.78	0.40
2:G:319:ARG:HG3	2:G:320:SER:N	2.36	0.40
1:J:350:ALA:C	1:J:352:ALA:H	2.26	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
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:12:ALA:C	3:Y:14:ARG:H	2.29	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:A:156:MET:HB2	3:A:156:MET:HE3	1.82	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1	R	220/240 (92%)	218 (99%)	1 (0%)	1 (0%)	25	47
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%)	25	47
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	21	43
1	C	164/177 (93%)	149 (91%)	15 (9%)	7	16
1	E	164/177 (93%)	151 (92%)	13 (8%)	10	21
1	H	164/177 (93%)	152 (93%)	12 (7%)	11	25
1	J	164/177 (93%)	153 (93%)	11 (7%)	13	29
1	L	164/177 (93%)	152 (93%)	12 (7%)	11	25
1	N	164/177 (93%)	154 (94%)	10 (6%)	15	34
1	P	164/177 (93%)	154 (94%)	10 (6%)	15	34
1	R	164/177 (93%)	152 (93%)	12 (7%)	11	25

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	T	164/177 (93%)	155 (94%)	9 (6%)	18 38
1	X	164/177 (93%)	153 (93%)	11 (7%)	13 29
1	Z	164/177 (93%)	150 (92%)	14 (8%)	8 18
2	G	165/178 (93%)	155 (94%)	10 (6%)	15 34
2	V	165/178 (93%)	153 (93%)	12 (7%)	11 25
3	1	163/184 (89%)	151 (93%)	12 (7%)	11 24
3	A	164/184 (89%)	149 (91%)	15 (9%)	7 16
3	B	165/184 (90%)	154 (93%)	11 (7%)	13 29
3	D	163/184 (89%)	144 (88%)	19 (12%)	4 8
3	F	162/184 (88%)	139 (86%)	23 (14%)	2 5
3	I	166/184 (90%)	158 (95%)	8 (5%)	21 44
3	K	165/184 (90%)	151 (92%)	14 (8%)	8 18
3	M	148/184 (80%)	137 (93%)	11 (7%)	11 24
3	O	164/184 (89%)	156 (95%)	8 (5%)	21 43
3	Q	163/184 (89%)	147 (90%)	16 (10%)	6 13
3	S	165/184 (90%)	151 (92%)	14 (8%)	8 18
3	U	162/184 (88%)	149 (92%)	13 (8%)	10 21
3	W	160/184 (87%)	144 (90%)	16 (10%)	6 13
3	Y	163/184 (89%)	152 (93%)	11 (7%)	13 29
All	All	4571/5056 (90%)	4221 (92%)	350 (8%)	10 22

All (350) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	303	ILE
1	H	322	GLN
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	444	LEU
1	H	461	ASP
1	H	471	LEU

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Mol	Chain	Res	Type
1	H	512	GLU
1	C	303	ILE
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	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	303	ILE
1	E	322	GLN
1	E	348	THR
1	E	351	VAL
1	E	362	GLU
1	E	363	LEU
1	E	374	LEU
1	E	433	GLU
1	E	434	GLU
1	E	444	LEU
1	E	461	ASP
1	E	471	LEU
1	E	519	GLU
2	G	303	ILE
2	G	322	GLN
2	G	345	ILE
2	G	362	GLU
2	G	363	LEU
2	G	433	GLU
2	G	444	LEU
2	G	461	ASP
2	G	471	LEU
2	G	512	GLU
1	J	303	ILE
1	J	322	GLN
1	J	348	THR

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Mol	Chain	Res	Type
1	J	362	GLU
1	J	374	LEU
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	303	ILE
1	L	322	GLN
1	L	362	GLU
1	L	363	LEU
1	L	374	LEU
1	L	396	GLN
1	L	433	GLU
1	L	444	LEU
1	L	461	ASP
1	L	471	LEU
1	L	503	VAL
1	L	515	ARG
1	N	303	ILE
1	N	322	GLN
1	N	362	GLU
1	N	363	LEU
1	N	374	LEU
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	303	ILE
1	R	322	GLN

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Mol	Chain	Res	Type
1	R	348	THR
1	R	353	VAL
1	R	362	GLU
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	R	512	GLU
1	T	303	ILE
1	T	322	GLN
1	T	362	GLU
1	T	363	LEU
1	T	374	LEU
1	T	433	GLU
1	T	444	LEU
1	T	471	LEU
1	T	503	VAL
2	V	301	THR
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	348	THR
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	513	LEU
1	X	519	GLU

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Mol	Chain	Res	Type
1	Z	303	ILE
1	Z	322	GLN
1	Z	354	GLU
1	Z	362	GLU
1	Z	363	LEU
1	Z	374	LEU
1	Z	396	GLN
1	Z	444	LEU
1	Z	461	ASP
1	Z	471	LEU
1	Z	503	VAL
1	Z	507	GLU
1	Z	508	SER
1	Z	519	GLU
1	2	322	GLN
1	2	362	GLU
1	2	363	LEU
1	2	374	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	73	ASN
3	D	74	LEU
3	D	90	ASP
3	D	93	ASP
3	D	99	LEU
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	178	THR
3	D	188	LEU
3	D	234	LEU
3	A	9	MET

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Mol	Chain	Res	Type
3	A	10	GLU
3	A	13	MET
3	A	33	LEU
3	A	73	ASN
3	A	74	LEU
3	A	102	VAL
3	A	107	LEU
3	A	170	SER
3	A	178	THR
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	99	LEU
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	18	GLU
3	F	21	ARG
3	F	24	ILE
3	F	73	ASN
3	F	74	LEU
3	F	84	THR
3	F	90	ASP
3	F	102	VAL
3	F	107	LEU
3	F	113	GLU
3	F	116	LYS
3	F	163	ILE
3	F	168	LYS

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Mol	Chain	Res	Type
3	F	174	ASN
3	F	178	THR
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	216	ASN
3	I	235	VAL
3	K	11	GLN
3	K	13	MET
3	K	21	ARG
3	K	73	ASN
3	K	74	LEU
3	K	99	LEU
3	K	107	LEU
3	K	112	THR
3	K	113	GLU
3	K	132	GLU
3	K	137	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	107	LEU
3	M	113	GLU
3	M	159	THR
3	M	170	SER
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

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Mol	Chain	Res	Type
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	99	LEU
3	Q	102	VAL
3	Q	107	LEU
3	Q	113	GLU
3	Q	159	THR
3	Q	161	GLU
3	Q	163	ILE
3	Q	173	GLU
3	Q	181	LEU
3	Q	188	LEU
3	Q	192	SER
3	Q	216	ASN
3	Q	234	LEU
3	S	9	MET
3	S	11	GLN
3	S	73	ASN
3	S	74	LEU
3	S	92	ARG
3	S	102	VAL
3	S	107	LEU
3	S	112	THR
3	S	163	ILE
3	S	178	THR
3	S	188	LEU
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	99	LEU
3	U	102	VAL
3	U	107	LEU

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Mol	Chain	Res	Type
3	U	149	ASP
3	U	159	THR
3	U	169	GLU
3	U	174	ASN
3	U	208	LEU
3	U	212	VAL
3	W	18	GLU
3	W	24	ILE
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	169	GLU
3	W	173	GLU
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	11	GLN
3	Y	13	MET
3	Y	59	ARG
3	Y	73	ASN
3	Y	74	LEU
3	Y	107	LEU
3	Y	113	GLU
3	Y	159	THR
3	Y	176	SER
3	Y	207	SER
3	Y	234	LEU
3	1	10	GLU
3	1	13	MET
3	1	73	ASN
3	1	74	LEU
3	1	99	LEU
3	1	102	VAL
3	1	107	LEU
3	1	113	GLU
3	1	159	THR

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Mol	Chain	Res	Type
3	1	185	VAL
3	1	205	VAL
3	1	234	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (81) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	390	ASN
1	H	410	HIS
1	E	390	ASN
1	E	410	HIS
1	E	456	GLN
2	G	381	ASN
1	J	410	HIS
1	L	390	ASN
1	N	390	ASN
1	N	437	GLN
1	P	390	ASN
1	X	456	GLN
1	Z	410	HIS
1	Z	430	ASN
1	2	381	ASN
1	2	410	HIS
3	D	69	ASN
3	D	101	ASN
3	D	114	GLN
3	D	216	ASN
3	A	69	ASN
3	A	73	ASN
3	A	98	GLN
3	A	101	ASN
3	A	105	GLN
3	A	114	GLN
3	A	129	HIS
3	B	69	ASN
3	B	101	ASN
3	F	69	ASN
3	F	98	GLN
3	F	105	GLN
3	F	152	HIS
3	F	174	ASN
3	I	51	GLN

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Mol	Chain	Res	Type
3	I	69	ASN
3	I	73	ASN
3	K	69	ASN
3	K	73	ASN
3	K	98	GLN
3	K	101	ASN
3	K	129	HIS
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	98	GLN
3	O	129	HIS
3	Q	69	ASN
3	Q	101	ASN
3	Q	114	GLN
3	Q	152	HIS
3	Q	174	ASN
3	S	69	ASN
3	S	98	GLN
3	S	114	GLN
3	S	174	ASN
3	S	231	GLN
3	U	69	ASN
3	U	80	GLN
3	U	101	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	Y	11	GLN
3	Y	69	ASN
3	Y	73	ASN
3	Y	114	GLN
3	Y	129	HIS
3	Y	174	ASN

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Mol	Chain	Res	Type
3	1	11	GLN
3	1	69	ASN
3	1	73	ASN
3	1	101	ASN

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	X	301	1	6,9,10	5.47	5 (83%)	9,12,14	5.82	7 (77%)
1	OZT	T	301	1	6,9,10	5.72	5 (83%)	9,12,14	5.52	7 (77%)
1	OZT	C	301	1	6,9,10	5.54	5 (83%)	9,12,14	5.95	6 (66%)
1	OZT	L	301	1	6,9,10	5.56	5 (83%)	9,12,14	5.94	6 (66%)
1	OZT	E	301	1	6,9,10	5.72	3 (50%)	9,12,14	5.82	7 (77%)
1	OZT	J	301	1	6,9,10	4.97	4 (66%)	9,12,14	6.14	7 (77%)
1	OZT	R	301	1	6,9,10	5.54	5 (83%)	9,12,14	5.96	6 (66%)
1	OZT	Z	301	1	6,9,10	6.10	5 (83%)	9,12,14	5.52	6 (66%)
1	OZT	N	301	1	6,9,10	5.00	5 (83%)	9,12,14	5.63	6 (66%)
1	OZT	H	301	1	6,9,10	5.66	5 (83%)	9,12,14	6.09	6 (66%)
1	OZT	2	301	1	6,9,10	4.77	4 (66%)	9,12,14	5.63	6 (66%)
1	OZT	P	301	1	6,9,10	6.57	4 (66%)	9,12,14	6.27	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	X	301	1	-	0/1/14/16	0/1/1/1
1	OZT	T	301	1	-	0/1/14/16	0/1/1/1
1	OZT	C	301	1	-	1/1/14/16	0/1/1/1
1	OZT	L	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	J	301	1	-	1/1/14/16	0/1/1/1
1	OZT	R	301	1	-	1/1/14/16	0/1/1/1
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	H	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	P	301	1	-	1/1/14/16	0/1/1/1

All (55) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	P	301	OZT	O1-C5	13.18	1.54	1.36
1	Z	301	OZT	O1-C5	12.79	1.53	1.36
1	E	301	OZT	O1-C5	11.62	1.52	1.36
1	H	301	OZT	O1-C5	11.45	1.51	1.36
1	J	301	OZT	O1-C5	10.76	1.50	1.36
1	X	301	OZT	O1-C5	10.63	1.50	1.36
1	L	301	OZT	O1-C5	10.57	1.50	1.36
1	R	301	OZT	O1-C5	10.56	1.50	1.36
1	C	301	OZT	O1-C5	10.52	1.50	1.36
1	T	301	OZT	O1-C5	10.32	1.50	1.36
1	2	301	OZT	O1-C5	10.28	1.50	1.36
1	N	301	OZT	C5-N	8.86	1.45	1.33
1	P	301	OZT	C5-N	7.47	1.43	1.33
1	T	301	OZT	C5-N	7.39	1.43	1.33
1	E	301	OZT	C5-N	6.90	1.43	1.33
1	L	301	OZT	C5-N	6.79	1.42	1.33
1	R	301	OZT	C5-N	6.76	1.42	1.33
1	C	301	OZT	C5-N	6.73	1.42	1.33
1	X	301	OZT	C5-N	6.69	1.42	1.33
1	N	301	OZT	O1-C5	6.67	1.45	1.36
1	Z	301	OZT	C5-N	5.36	1.40	1.33
1	H	301	OZT	C5-N	5.10	1.40	1.33
1	T	301	OZT	O6-C5	4.33	1.29	1.21
1	H	301	OZT	O1-C2	-4.14	1.40	1.46
1	C	301	OZT	O1-C2	-4.00	1.40	1.46
1	Z	301	OZT	O1-C2	-3.99	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	P	301	OZT	O6-C5	3.97	1.29	1.21
1	L	301	OZT	O1-C2	-3.97	1.40	1.46
1	R	301	OZT	O1-C2	-3.92	1.40	1.46
1	J	301	OZT	O1-C2	-3.66	1.41	1.46
1	H	301	OZT	C7-C2	-3.54	1.43	1.51
1	N	301	OZT	O1-C2	-3.52	1.41	1.46
1	2	301	OZT	O1-C2	-3.50	1.41	1.46
1	T	301	OZT	O1-C2	-3.44	1.41	1.46
1	X	301	OZT	O1-C2	-3.36	1.41	1.46
1	2	301	OZT	C5-N	3.36	1.38	1.33
1	J	301	OZT	C5-N	3.36	1.38	1.33
1	P	301	OZT	O1-C2	-3.11	1.41	1.46
1	Z	301	OZT	O6-C5	3.05	1.27	1.21
1	N	301	OZT	O6-C5	2.69	1.26	1.21
1	N	301	OZT	C7-C2	-2.61	1.45	1.51
1	C	301	OZT	C7-C2	-2.56	1.45	1.51
1	L	301	OZT	C7-C2	-2.55	1.45	1.51
1	R	301	OZT	C7-C2	-2.54	1.45	1.51
1	E	301	OZT	O6-C5	2.54	1.26	1.21
1	J	301	OZT	C7-C2	-2.53	1.45	1.51
1	X	301	OZT	O6-C5	2.44	1.26	1.21
1	Z	301	OZT	C7-C2	-2.15	1.46	1.51
1	H	301	OZT	O6-C5	2.15	1.25	1.21
1	C	301	OZT	O6-C5	2.14	1.25	1.21
1	R	301	OZT	O6-C5	2.11	1.25	1.21
1	L	301	OZT	O6-C5	2.11	1.25	1.21
1	T	301	OZT	C7-C2	-2.04	1.46	1.51
1	X	301	OZT	C7-C2	-2.02	1.46	1.51
1	2	301	OZT	C7-C2	-2.02	1.46	1.51

All (77) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	J	301	OZT	O1-C5-N	9.55	117.65	109.87
1	P	301	OZT	O1-C2-CA	9.29	112.17	103.72
1	R	301	OZT	O1-C5-N	8.72	116.97	109.87
1	C	301	OZT	O1-C5-N	8.71	116.97	109.87
1	L	301	OZT	O1-C5-N	8.67	116.94	109.87
1	H	301	OZT	O1-C5-N	8.63	116.90	109.87
1	T	301	OZT	O1-C2-CA	8.59	111.53	103.72
1	2	301	OZT	O1-C5-N	8.57	116.85	109.87
1	R	301	OZT	CA-N-C5	-8.26	99.98	112.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	L	301	OZT	CA-N-C5	-8.25	99.99	112.75
1	C	301	OZT	CA-N-C5	-8.24	100.02	112.75
1	N	301	OZT	O1-C5-N	8.24	116.58	109.87
1	H	301	OZT	CA-N-C5	-8.23	100.03	112.75
1	X	301	OZT	O1-C2-CA	8.19	111.17	103.72
1	P	301	OZT	CA-N-C5	-8.18	100.11	112.75
1	Z	301	OZT	CA-N-C5	-8.11	100.21	112.75
1	X	301	OZT	O1-C5-N	8.07	116.44	109.87
1	E	301	OZT	O1-C5-N	8.05	116.43	109.87
1	N	301	OZT	O1-C2-CA	8.04	111.03	103.72
1	P	301	OZT	C2-O1-C5	-8.02	98.44	110.33
1	X	301	OZT	CA-N-C5	-7.93	100.50	112.75
1	J	301	OZT	CA-N-C5	-7.92	100.51	112.75
1	2	301	OZT	CA-N-C5	-7.90	100.54	112.75
1	N	301	OZT	CA-N-C5	-7.77	100.74	112.75
1	E	301	OZT	O1-C2-CA	7.73	110.75	103.72
1	E	301	OZT	CA-N-C5	-7.66	100.91	112.75
1	E	301	OZT	C2-O1-C5	-7.58	99.10	110.33
1	Z	301	OZT	O1-C5-N	7.44	115.93	109.87
1	P	301	OZT	O1-C5-N	7.43	115.92	109.87
1	J	301	OZT	O6-C5-N	-7.40	120.43	129.19
1	T	301	OZT	CA-N-C5	-7.33	101.43	112.75
1	X	301	OZT	C2-O1-C5	-7.27	99.55	110.33
1	J	301	OZT	C2-O1-C5	-7.26	99.57	110.33
1	H	301	OZT	C2-O1-C5	-7.21	99.64	110.33
1	T	301	OZT	O1-C5-N	7.17	115.72	109.87
1	C	301	OZT	O1-C2-CA	7.11	110.19	103.72
1	H	301	OZT	O1-C2-CA	7.10	110.18	103.72
1	R	301	OZT	O1-C2-CA	7.08	110.16	103.72
1	L	301	OZT	O1-C2-CA	7.07	110.15	103.72
1	T	301	OZT	C2-O1-C5	-6.87	100.15	110.33
1	Z	301	OZT	C2-O1-C5	-6.80	100.25	110.33
1	R	301	OZT	C2-O1-C5	-6.74	100.34	110.33
1	H	301	OZT	C2-CA-C	-6.73	104.80	114.16
1	2	301	OZT	C2-O1-C5	-6.72	100.37	110.33
1	C	301	OZT	C2-O1-C5	-6.72	100.38	110.33
1	R	301	OZT	C2-CA-C	-6.71	104.83	114.16
1	L	301	OZT	C2-O1-C5	-6.71	100.39	110.33
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	2	301	OZT	O6-C5-N	-6.66	121.31	129.19
1	Z	301	OZT	O1-C2-CA	6.53	109.66	103.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	J	301	OZT	O1-C2-CA	6.52	109.65	103.72
1	H	301	OZT	O6-C5-N	-6.37	121.65	129.19
1	P	301	OZT	O6-C5-N	-6.30	121.73	129.19
1	Z	301	OZT	O6-C5-N	-6.16	121.90	129.19
1	E	301	OZT	O6-C5-N	-6.15	121.91	129.19
1	2	301	OZT	O1-C2-CA	6.15	109.31	103.72
1	N	301	OZT	C2-O1-C5	-6.14	101.23	110.33
1	P	301	OZT	C2-CA-C	-5.94	105.90	114.16
1	N	301	OZT	C2-CA-C	-5.92	105.93	114.16
1	R	301	OZT	O6-C5-N	-5.57	122.59	129.19
1	X	301	OZT	O6-C5-N	-5.57	122.60	129.19
1	J	301	OZT	C2-CA-C	-5.55	106.44	114.16
1	C	301	OZT	O6-C5-N	-5.55	122.63	129.19
1	L	301	OZT	O6-C5-N	-5.55	122.63	129.19
1	T	301	OZT	O6-C5-N	-4.96	123.33	129.19
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	T	301	OZT	C2-CA-C	-4.18	108.34	114.16
1	N	301	OZT	O6-C5-N	-3.29	125.30	129.19
1	X	301	OZT	O-C-CA	-2.51	118.22	124.86
1	E	301	OZT	O-C-CA	-2.25	118.90	124.86
1	T	301	OZT	O-C-CA	-2.20	119.05	124.86
1	P	301	OZT	O-C-CA	-2.17	119.11	124.86
1	J	301	OZT	O-C-CA	-2.09	119.34	124.86

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
1	2	301	OZT	O-C-CA-C2

There are no ring outliers.

12 monomers are involved in 65 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	X	301	OZT	7	0
1	T	301	OZT	6	0
1	C	301	OZT	6	0
1	L	301	OZT	4	0
1	E	301	OZT	5	0
1	J	301	OZT	4	0
1	R	301	OZT	5	0
1	Z	301	OZT	7	0
1	N	301	OZT	2	0
1	H	301	OZT	6	0
1	2	301	OZT	6	0
1	P	301	OZT	7	0

5.5 Carbohydrates (i)

There are no oligosaccharides 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

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	2	221/240 (92%)	-0.23	1 (0%)	87	84	14, 40, 80, 106	0
1	C	221/240 (92%)	-0.08	4 (1%)	67	62	16, 46, 84, 106	0
1	E	221/240 (92%)	-0.15	3 (1%)	73	68	22, 45, 81, 114	0
1	H	221/240 (92%)	-0.31	4 (1%)	67	62	14, 37, 86, 102	0
1	J	221/240 (92%)	-0.14	4 (1%)	67	62	17, 45, 86, 111	0
1	L	221/240 (92%)	-0.38	2 (0%)	81	77	10, 37, 82, 110	0
1	N	221/240 (92%)	-0.43	6 (2%)	56	50	6, 28, 85, 120	0
1	P	221/240 (92%)	-0.40	7 (3%)	50	45	10, 29, 78, 109	0
1	R	221/240 (92%)	-0.09	1 (0%)	87	84	21, 48, 89, 115	0
1	T	221/240 (92%)	-0.08	5 (2%)	61	55	12, 42, 84, 120	0
1	X	221/240 (92%)	-0.16	4 (1%)	67	62	16, 38, 80, 116	0
1	Z	221/240 (92%)	-0.06	2 (0%)	81	77	21, 48, 84, 111	0
2	G	222/240 (92%)	-0.09	3 (1%)	73	68	11, 45, 79, 109	0
2	V	224/240 (93%)	-0.36	7 (3%)	51	46	9, 30, 79, 108	0
3	1	213/240 (88%)	0.57	13 (6%)	28	23	27, 70, 104, 115	0
3	A	214/240 (89%)	0.00	3 (1%)	73	68	7, 45, 85, 101	0
3	B	216/240 (90%)	0.05	7 (3%)	50	45	6, 40, 85, 102	0
3	D	213/240 (88%)	0.61	12 (5%)	31	25	19, 70, 102, 125	0
3	F	212/240 (88%)	0.34	16 (7%)	22	17	16, 55, 128, 161	0
3	I	217/240 (90%)	-0.02	1 (0%)	87	84	15, 44, 83, 101	0
3	K	216/240 (90%)	0.25	4 (1%)	66	61	18, 60, 94, 115	0
3	M	194/240 (80%)	0.54	13 (6%)	25	20	26, 73, 103, 116	0
3	O	214/240 (89%)	0.20	7 (3%)	49	43	16, 55, 93, 106	0
3	Q	213/240 (88%)	0.73	17 (7%)	20	16	27, 70, 108, 130	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
3	S	215/240 (89%)	0.21	5 (2%) 61 55	17, 56, 95, 113	0
3	U	212/240 (88%)	1.05	38 (17%) 4 3	20, 76, 105, 120	0
3	W	209/240 (87%)	0.50	6 (2%) 54 48	25, 66, 99, 112	0
3	Y	213/240 (88%)	0.34	5 (2%) 61 55	19, 62, 97, 114	0
All	All	6069/6720 (90%)	0.08	200 (3%) 49 43	6, 49, 95, 161	0

All (200) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	V	349	ALA	5.4
1	P	353	VAL	4.7
1	H	349	ALA	4.6
3	W	205	VAL	4.3
1	X	425	ALA	4.2
3	U	141	ILE	4.2
3	U	234	LEU	4.2
3	W	208	LEU	4.0
3	Y	205	VAL	3.9
2	V	524	ALA	3.9
3	Q	33	LEU	3.9
1	T	349	ALA	3.8
3	Q	234	LEU	3.8
3	U	188	LEU	3.6
1	H	347	GLY	3.6
3	U	184	ALA	3.6
1	H	353	VAL	3.5
3	Q	172	ALA	3.5
2	G	350	ALA	3.5
2	V	352	ALA	3.4
1	E	425	ALA	3.4
3	1	183	ILE	3.4
1	2	351	VAL	3.3
3	K	186	ALA	3.3
3	Q	190	ALA	3.2
1	C	353	VAL	3.2
3	Q	188	LEU	3.2
1	X	355	PHE	3.2
1	C	349	ALA	3.2
1	T	350	ALA	3.2
1	N	427	GLY	3.2
3	U	183	ILE	3.2

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Mol	Chain	Res	Type	RSRZ
3	B	133	THR	3.2
3	U	181	LEU	3.2
3	U	154	VAL	3.1
3	F	15	GLU	3.1
3	U	167	LEU	3.1
2	G	347	GLY	3.1
3	1	188	LEU	3.1
3	F	22	LYS	3.1
3	F	159	THR	3.0
1	E	398	LEU	3.0
3	U	233	LEU	3.0
3	F	14	ARG	3.0
1	N	400	ALA	3.0
3	Q	32	ALA	3.0
3	U	33	LEU	2.9
1	P	425	ALA	2.9
3	U	227	GLY	2.9
3	S	12	ALA	2.8
3	1	36	ALA	2.8
3	1	153	PHE	2.8
3	D	186	ALA	2.8
3	U	175	ALA	2.8
3	U	172	ALA	2.8
3	U	124	VAL	2.8
1	J	349	ALA	2.8
3	M	232	ALA	2.8
3	U	180	ALA	2.8
1	J	351	VAL	2.7
1	P	349	ALA	2.7
1	T	348	THR	2.7
3	U	12	ALA	2.7
3	U	143	TYR	2.7
3	U	185	VAL	2.7
3	Y	36	ALA	2.7
1	N	398	LEU	2.7
3	U	225	ILE	2.7
1	X	399	LEU	2.7
2	V	350	ALA	2.7
3	M	159	THR	2.7
3	U	226	THR	2.7
3	F	20	ALA	2.6
3	M	188	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	H	351	VAL	2.6
3	Q	187	ALA	2.6
1	E	347	GLY	2.6
3	U	120	VAL	2.6
3	W	19	LEU	2.6
3	F	205	VAL	2.6
3	Q	42	VAL	2.6
3	S	205	VAL	2.6
3	M	51	GLN	2.6
3	U	24	ILE	2.6
3	D	234	LEU	2.5
1	J	352	ALA	2.5
3	Q	34	ALA	2.5
3	U	139	TYR	2.5
1	P	351	VAL	2.5
3	1	171	TYR	2.5
3	O	235	VAL	2.5
1	L	392	ALA	2.5
3	D	172	ALA	2.5
3	Y	190	ALA	2.5
3	1	12	ALA	2.5
2	V	348	THR	2.5
1	C	350	ALA	2.4
1	L	425	ALA	2.4
3	1	175	ALA	2.4
3	Q	177	LEU	2.4
3	D	13	MET	2.4
3	Q	205	VAL	2.4
3	M	71	PHE	2.4
3	Q	153	PHE	2.4
1	P	352	ALA	2.4
3	U	32	ALA	2.4
3	W	159	THR	2.4
3	F	19	LEU	2.4
3	D	182	ARG	2.4
3	B	21	ARG	2.4
3	O	205	VAL	2.4
3	F	25	ALA	2.4
3	M	172	ALA	2.4
3	U	34	ALA	2.4
3	U	191	GLY	2.4
2	G	348	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	N	425	ALA	2.3
3	A	188	LEU	2.3
3	F	21	ARG	2.3
1	P	355	PHE	2.3
3	Q	225	ILE	2.3
3	B	191	GLY	2.3
3	D	10	GLU	2.3
3	U	230	LEU	2.3
3	Y	234	LEU	2.3
3	F	18	GLU	2.3
3	M	184	ALA	2.3
3	U	206	ALA	2.3
3	O	188	LEU	2.3
3	Q	192	SER	2.3
3	Q	159	THR	2.2
3	1	149	ASP	2.2
3	D	153	PHE	2.2
3	F	12	ALA	2.2
1	J	347	GLY	2.2
3	I	203	LEU	2.2
3	U	121	GLU	2.2
3	D	151	PRO	2.2
3	U	162	PRO	2.2
3	W	171	TYR	2.2
3	K	93	ASP	2.2
1	Z	425	ALA	2.2
3	D	190	ALA	2.2
3	M	230	LEU	2.2
3	1	167	LEU	2.2
3	D	143	TYR	2.2
3	F	11	GLN	2.2
1	N	393	ALA	2.2
3	A	190	ALA	2.2
3	B	164	ALA	2.2
3	O	190	ALA	2.2
3	F	17	SER	2.2
3	D	110	ILE	2.2
1	X	398	LEU	2.2
3	A	234	LEU	2.2
3	B	131	GLY	2.2
3	U	165	ASN	2.1
1	T	351	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	T	415	GLN	2.1
1	Z	355	PHE	2.1
3	U	163	ILE	2.1
3	M	27	ALA	2.1
3	U	166	ALA	2.1
3	U	211	ALA	2.1
3	F	28	LYS	2.1
3	O	233	LEU	2.1
3	S	92	ARG	2.1
3	Y	172	ALA	2.1
3	U	160	THR	2.1
3	1	31	VAL	2.1
3	D	12	ALA	2.1
3	B	232	ALA	2.1
3	O	206	ALA	2.1
3	U	186	ALA	2.1
3	M	191	GLY	2.1
3	M	67	LYS	2.1
3	Q	160	THR	2.1
3	B	192	SER	2.1
1	N	391	LEU	2.1
3	F	143	TYR	2.1
3	Q	171	TYR	2.1
1	C	332	ARG	2.1
1	R	349	ALA	2.1
3	O	12	ALA	2.1
3	U	232	ALA	2.1
2	V	347	GLY	2.1
3	S	9	MET	2.0
3	M	192	SER	2.0
3	M	205	VAL	2.0
3	S	207	SER	2.0
3	K	143	TYR	2.0
1	P	350	ALA	2.0
3	1	187	ALA	2.0
2	V	523	GLY	2.0
3	F	13	MET	2.0
3	W	167	LEU	2.0
3	1	19	LEU	2.0
3	1	42	VAL	2.0
3	U	140	ARG	2.0
3	K	190	ALA	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^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	OZT	Z	301	9/10	0.83	0.13	36,41,47,48	0
1	OZT	R	301	9/10	0.84	0.13	63,65,66,68	0
1	OZT	T	301	9/10	0.86	0.14	31,38,44,46	0
1	OZT	C	301	9/10	0.86	0.16	72,76,77,78	0
1	OZT	P	301	9/10	0.90	0.11	34,41,46,47	0
1	OZT	H	301	9/10	0.90	0.11	35,41,45,46	0
1	OZT	E	301	9/10	0.90	0.12	36,42,46,48	0
1	OZT	J	301	9/10	0.90	0.09	34,38,40,41	0
1	OZT	L	301	9/10	0.91	0.10	27,33,36,37	0
1	OZT	2	301	9/10	0.91	0.10	31,34,39,43	0
1	OZT	X	301	9/10	0.94	0.08	24,28,31,32	0
1	OZT	N	301	9/10	0.96	0.07	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.