



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2018 – 04:41 pm GMT

PDB ID : 5D4Z  
Title : Crystal structure of Repressor from Salmonella-temperate phage  
Authors : Kim, H.J.; Yoon, H.J.; Ryu, S.; Lee, H.H.  
Deposited on : 2015-08-10  
Resolution : 2.98 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

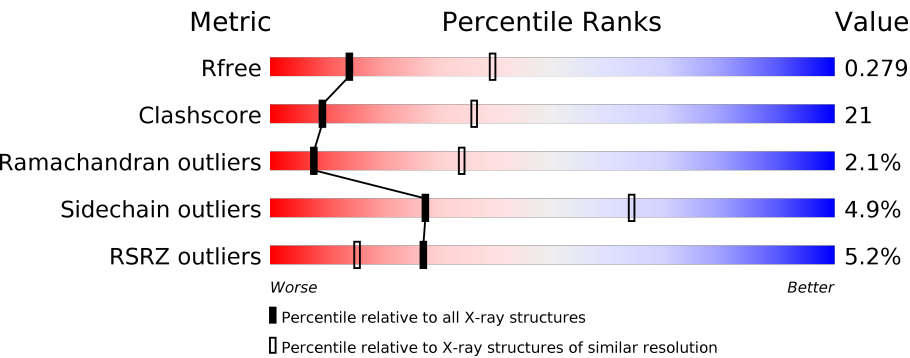
MolProbity : 4.02b-467  
Xtriage (Phenix) : 1.13  
EDS : trunk30967  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk30967

# 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 2.98 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.



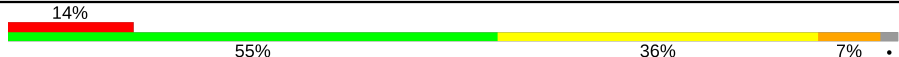




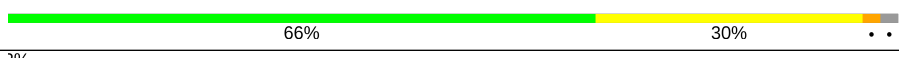
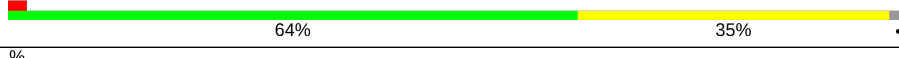
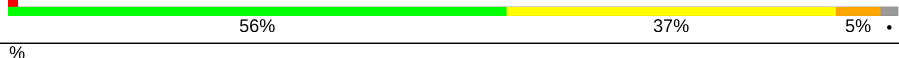







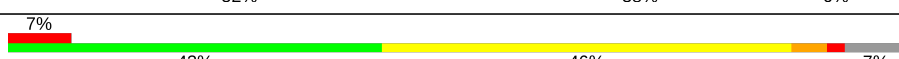
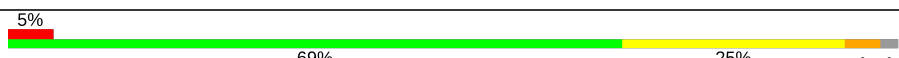
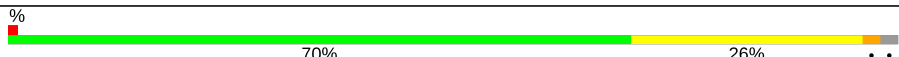
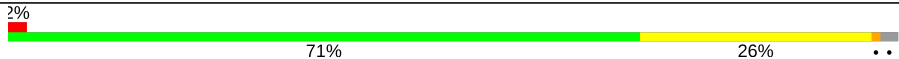




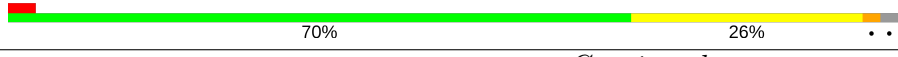

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	111664	2374 (3.00-2.96)
Clashscore	122126	2712 (3.00-2.96)
Ramachandran outliers	120053	2626 (3.00-2.96)
Sidechain outliers	120020	2629 (3.00-2.96)
RSRZ outliers	108989	2268 (3.00-2.96)

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

Mol	Chain	Length	Quality of chain
1	1	107	<div><div>3%</div><div><div></div><div>50%</div><div>48%</div><div>..</div></div></div>
1	2	107	<div><div>8%</div><div><div></div><div>57%</div><div>34%</div><div>6%</div></div></div>
1	3	107	<div><div>2%</div><div><div></div><div>50%</div><div>38%</div><div>5%</div><div>7%</div></div></div>
1	4	107	<div><div>17%</div><div><div></div><div>48%</div><div>45%</div><div>7%</div></div></div>
1	5	107	<div><div>7%</div><div><div></div><div>48%</div><div>41%</div><div>7%</div></div></div>
1	6	107	<div><div>17%</div><div><div></div><div>50%</div><div>33%</div><div>11%</div><div>6%</div></div></div>

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Mol	Chain	Length	Quality of chain
1	7	107	
1	A	107	
1	B	107	
1	C	107	
1	D	107	
1	E	107	
1	F	107	
1	G	107	
1	H	107	
1	I	107	
1	J	107	
1	K	107	
1	L	107	
1	M	107	
1	N	107	
1	O	107	
1	P	107	
1	Q	107	
1	R	107	
1	T	107	
1	U	107	
1	V	107	
1	W	107	
1	X	107	
1	Y	107	

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Mol	Chain	Length	Quality of chain
1	Z	107	<div><div></div><div>13%</div><div>47%</div><div>38%</div><div>8%</div><div>7%</div></div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 25962 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 Repressor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	105	Total	C	N	O	S	0	0	0
			808	513	138	152	5			
1	B	105	Total	C	N	O	S	0	0	0
			808	513	138	152	5			
1	C	105	Total	C	N	O	S	0	0	0
			808	513	138	152	5			
1	D	101	Total	C	N	O	S	0	0	0
			773	493	131	144	5			
1	E	105	Total	C	N	O	S	0	0	0
			808	513	138	152	5			
1	F	105	Total	C	N	O	S	0	0	0
			808	513	138	152	5			
1	G	105	Total	C	N	O	S	0	0	0
			808	513	138	152	5			
1	H	102	Total	C	N	O	S	0	0	0
			782	498	132	147	5			
1	I	105	Total	C	N	O	S	0	0	0
			808	513	138	152	5			
1	J	103	Total	C	N	O	S	0	0	0
			791	503	134	149	5			
1	K	105	Total	C	N	O	S	0	0	0
			808	513	138	152	5			
1	L	105	Total	C	N	O	S	0	0	0
			808	513	138	152	5			
1	M	105	Total	C	N	O	S	0	0	0
			808	513	138	152	5			
1	N	102	Total	C	N	O	S	0	0	0
			782	498	132	147	5			
1	O	105	Total	C	N	O	S	0	0	0
			808	513	138	152	5			
1	P	100	Total	C	N	O	S	0	0	0
			762	484	130	143	5			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	105	Total	C	N	O	S	0	0	0
			808	513	138	152	5			
1	R	105	Total	C	N	O	S	0	0	0
			808	513	138	152	5			
1	T	105	Total	C	N	O	S	0	0	0
			808	513	138	152	5			
1	U	103	Total	C	N	O	S	0	0	0
			791	503	134	149	5			
1	V	105	Total	C	N	O	S	0	0	0
			808	513	138	152	5			
1	W	105	Total	C	N	O	S	0	0	0
			808	513	138	152	5			
1	X	105	Total	C	N	O	S	0	0	0
			808	513	138	152	5			
1	Y	105	Total	C	N	O	S	0	0	0
			808	513	138	152	5			
1	Z	100	Total	C	N	O	S	0	0	0
			762	484	130	143	5			
1	1	105	Total	C	N	O	S	0	0	0
			808	513	138	152	5			
1	2	101	Total	C	N	O	S	0	0	0
			773	493	131	144	5			
1	3	100	Total	C	N	O	S	0	0	0
			762	484	130	143	5			
1	4	100	Total	C	N	O	S	0	0	0
			762	484	130	143	5			
1	5	100	Total	C	N	O	S	0	0	0
			762	484	130	143	5			
1	6	101	Total	C	N	O	S	0	0	0
			773	493	131	144	5			
1	7	105	Total	C	N	O	S	0	0	0
			808	513	138	152	5			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	21	Total	O	0	0
			21	21		
2	B	24	Total	O	0	0
			24	24		
2	C	25	Total	O	0	0
			25	25		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	D	39	Total O 39 39	0	0
2	E	21	Total O 21 21	0	0
2	F	30	Total O 30 30	0	0
2	G	19	Total O 19 19	0	0
2	H	26	Total O 26 26	0	0
2	I	3	Total O 3 3	0	0
2	J	10	Total O 10 10	0	0
2	K	5	Total O 5 5	0	0
2	L	17	Total O 17 17	0	0
2	M	5	Total O 5 5	0	0
2	N	13	Total O 13 13	0	0
2	O	3	Total O 3 3	0	0
2	P	8	Total O 8 8	0	0
2	Q	18	Total O 18 18	0	0
2	R	33	Total O 33 33	0	0
2	T	32	Total O 32 32	0	0
2	U	27	Total O 27 27	0	0
2	V	16	Total O 16 16	0	0
2	W	27	Total O 27 27	0	0
2	X	19	Total O 19 19	0	0
2	Y	17	Total O 17 17	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	Z	4	Total 4	O 4	0	0
2	1	8	Total 8	O 8	0	0
2	2	7	Total 7	O 7	0	0
2	3	18	Total 18	O 18	0	0
2	4	6	Total 6	O 6	0	0
2	5	14	Total 14	O 14	0	0
2	6	3	Total 3	O 3	0	0
2	7	9	Total 9	O 9	0	0



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

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

- Molecule 1: Repressor



- Molecule 1: Repressor



- Molecule 1: Repressor



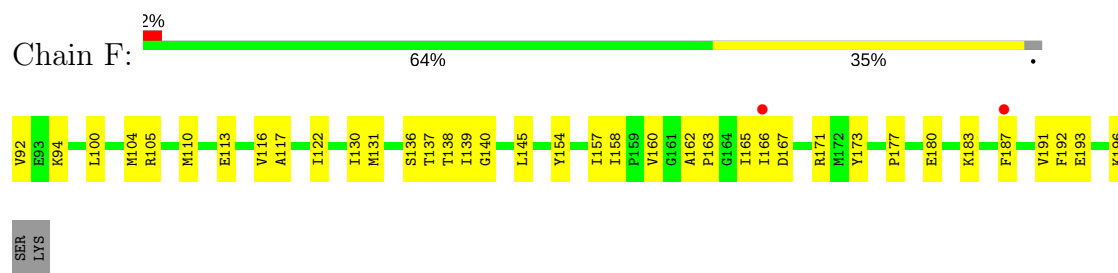
- Molecule 1: Repressor



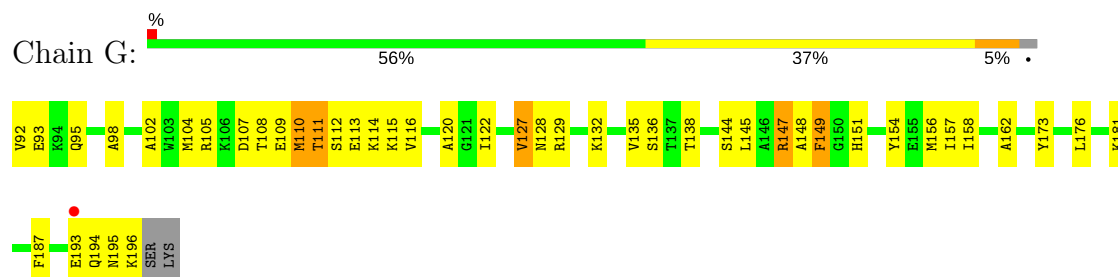
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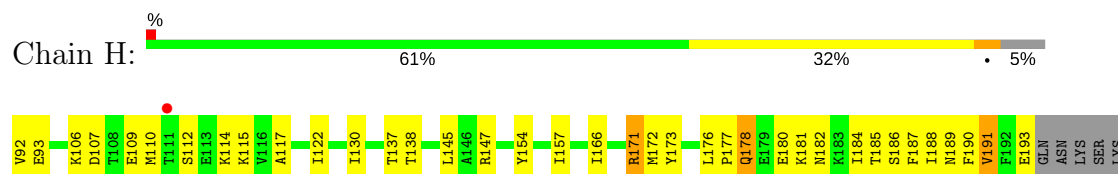
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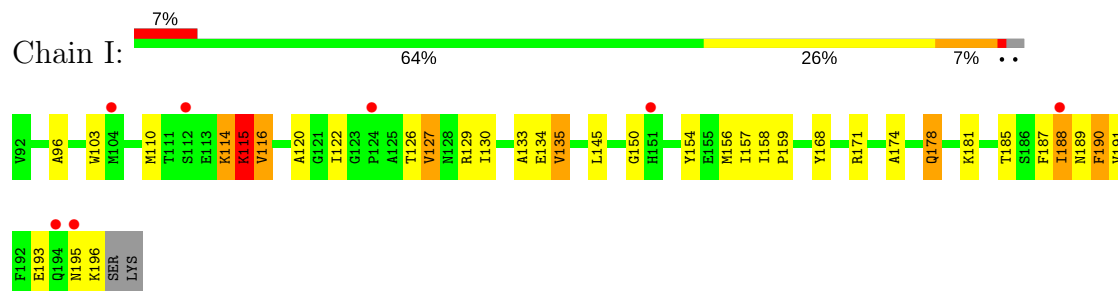
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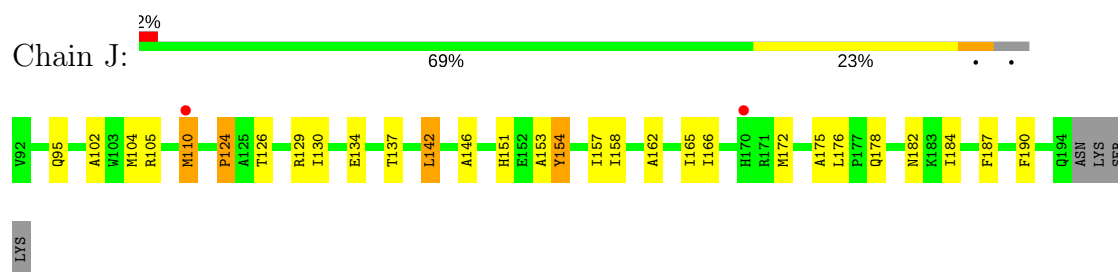
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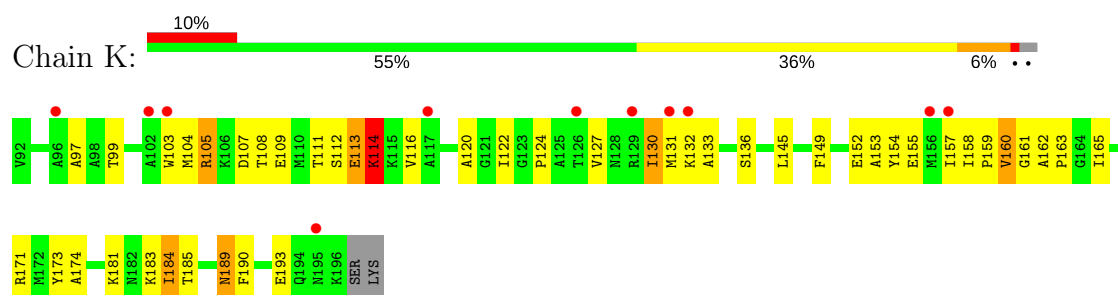
- Molecule 1: Repressor



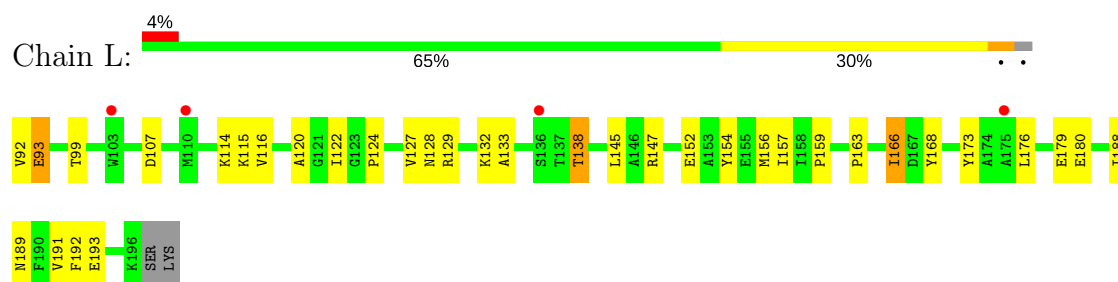
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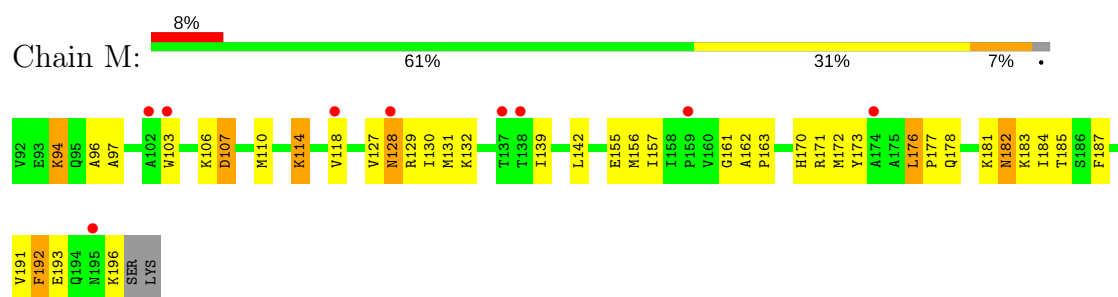
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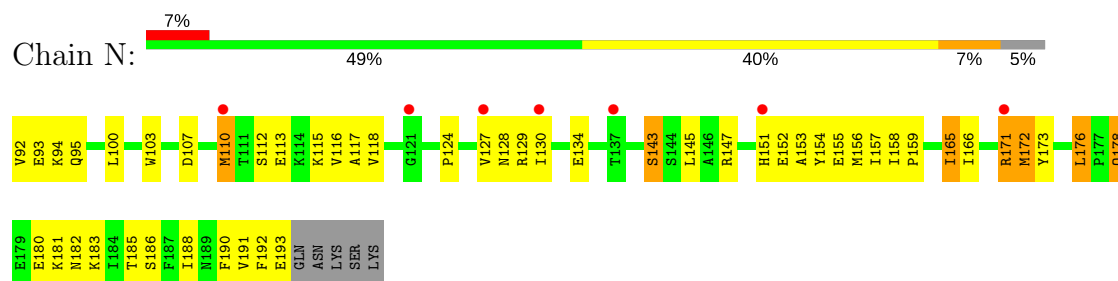
• Molecule 1: Repressor



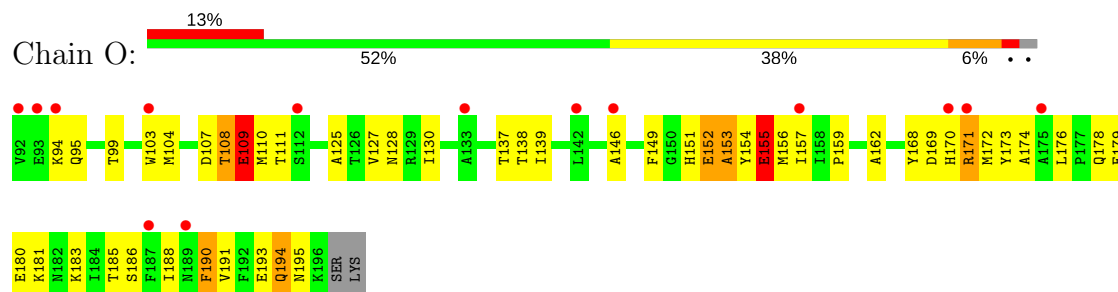
• Molecule 1: Repressor



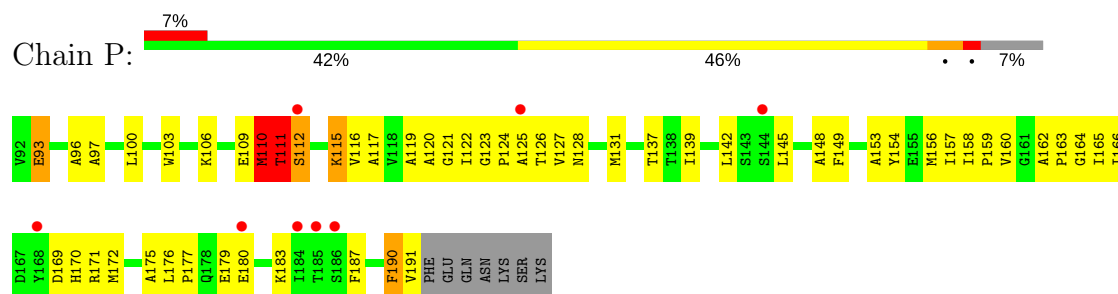
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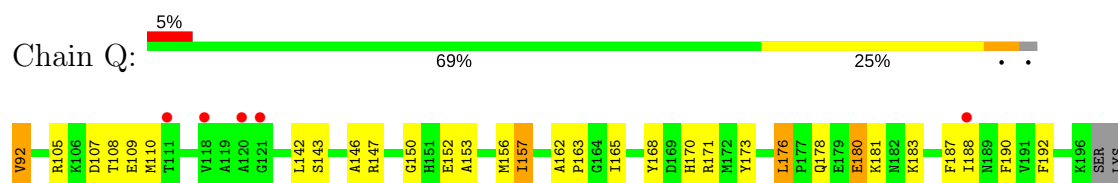
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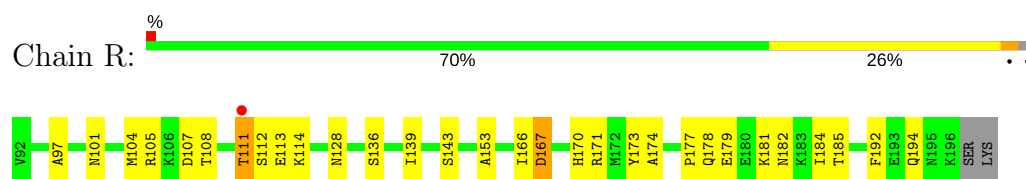
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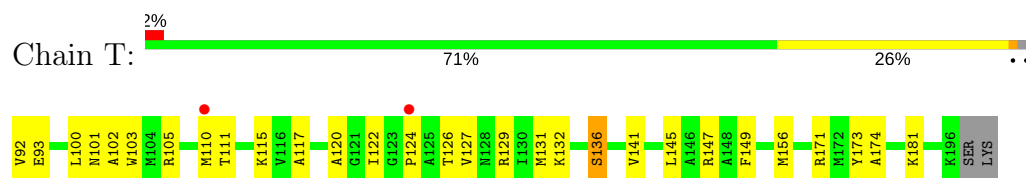
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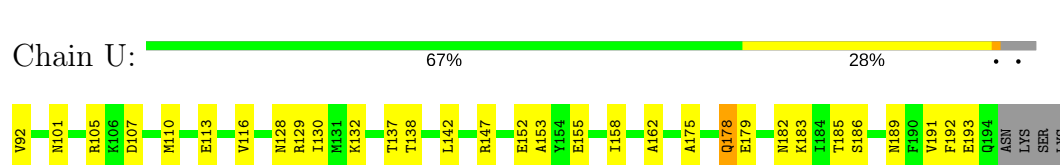
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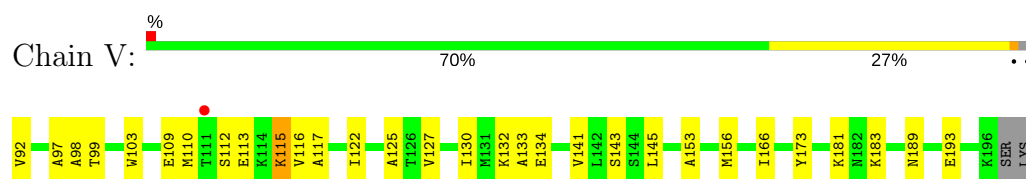
- Molecule 1: Repressor



- Molecule 1: Repressor



- Molecule 1: Repressor

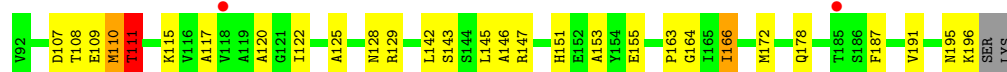


- Molecule 1: Repressor





• Molecule 1: Repressor



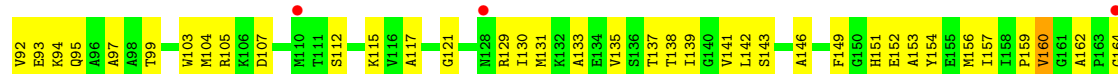
• Molecule 1: Repressor



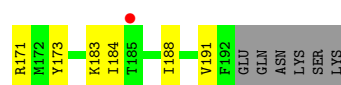
• Molecule 1: Repressor



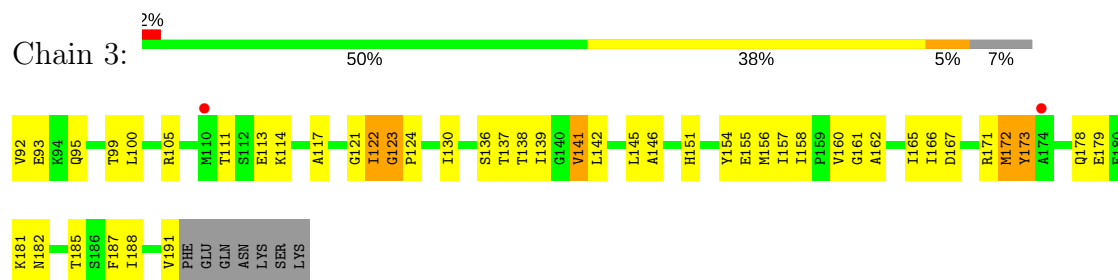
• Molecule 1: Repressor



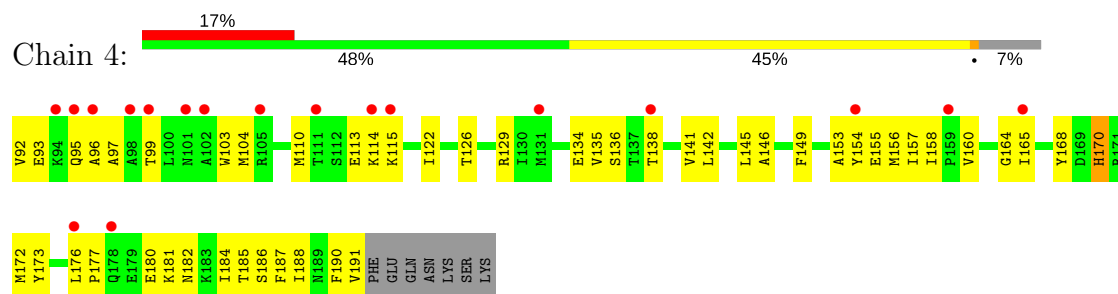
• Molecule 1: Repressor



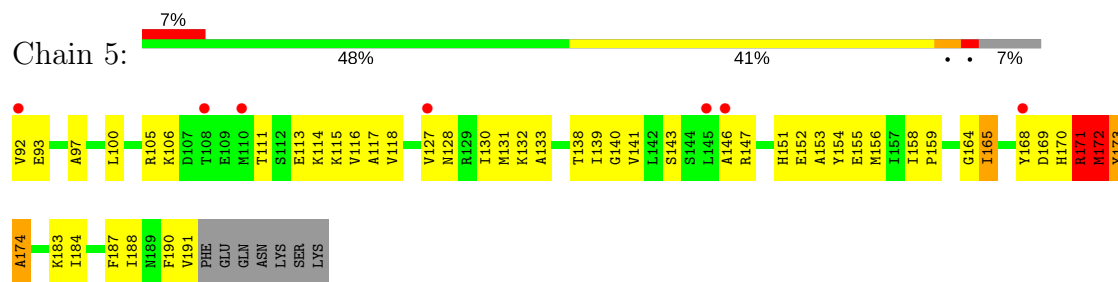
• Molecule 1: Repressor



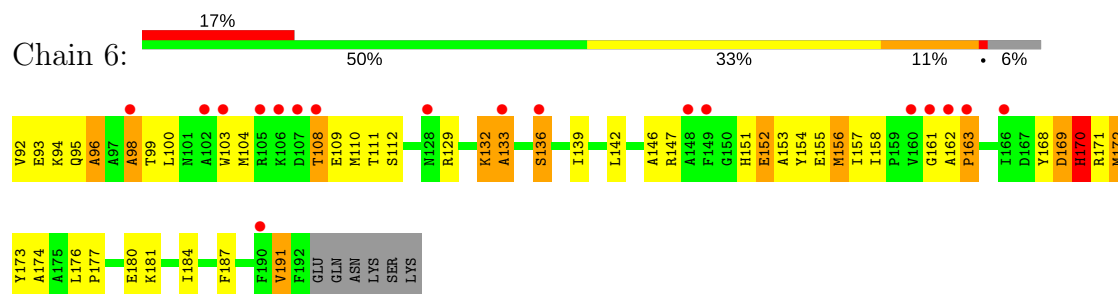
- Molecule 1: Repressor



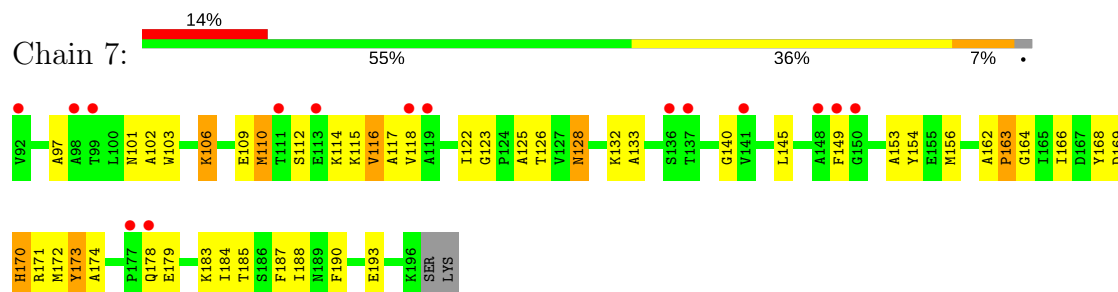
- Molecule 1: Repressor



- Molecule 1: Repressor



- Molecule 1: Repressor



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	61.60Å 62.50Å 267.90Å 89.99° 89.97° 72.70°	Depositor
Resolution (Å)	49.13 – 2.98 49.13 – 2.98	Depositor EDS
% Data completeness (in resolution range)	97.5 (49.13-2.98) 98.8 (49.13-2.98)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.43 (at 2.96Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, $R_{free}$	0.216 , 0.273 0.228 , 0.279	Depositor DCC
$R_{free}$ test set	3858 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	70.5	Xtriage
Anisotropy	0.028	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 97.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.53$ , $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	0.069 for -h,-k,l 0.001 for k,h,-l 0.002 for -k,-h,-l	Xtriage
Reported twinning fraction	0.509 for H, K, L 0.491 for -h,-k,l	Depositor
Outliers	0 of 76987 reflections	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	25962	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.46% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	1	0.38	0/822	0.61	0/1110
1	2	0.35	0/787	0.63	0/1064
1	3	0.34	0/775	0.62	0/1048
1	4	0.34	0/775	0.63	0/1048
1	5	0.37	0/775	0.62	0/1048
1	6	0.40	0/787	0.69	0/1064
1	7	0.42	0/822	0.73	0/1110
1	A	0.35	0/822	0.58	0/1110
1	B	0.38	0/822	0.59	0/1110
1	C	0.37	0/822	0.59	0/1110
1	D	0.38	0/787	0.60	0/1064
1	E	0.34	0/822	0.55	0/1110
1	F	0.38	0/822	0.58	0/1110
1	G	0.36	0/822	0.64	0/1110
1	H	0.40	0/796	0.61	0/1076
1	I	0.35	0/822	0.62	0/1110
1	J	0.35	0/805	0.56	0/1088
1	K	0.38	0/822	0.65	0/1110
1	L	0.36	0/822	0.65	0/1110
1	M	0.39	0/822	0.66	0/1110
1	N	0.38	0/796	0.64	0/1076
1	O	0.35	0/822	0.62	0/1110
1	P	0.39	0/775	0.65	0/1048
1	Q	0.37	0/822	0.57	0/1110
1	R	0.37	0/822	0.58	0/1110
1	T	0.35	0/822	0.62	0/1110
1	U	0.38	0/805	0.59	0/1088
1	V	0.37	0/822	0.59	0/1110
1	W	0.39	0/822	0.63	1/1110 (0.1%)
1	X	0.38	0/822	0.63	0/1110
1	Y	0.38	0/822	0.62	0/1110
1	Z	0.38	0/775	0.70	0/1048
All	All	0.37	0/25878	0.62	1/34960 (0.0%)



Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	2	0	2
1	5	0	1
1	6	0	2
1	7	0	1
1	O	0	1
All	All	0	7

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	W	105	ARG	NE-CZ-NH1	5.57	123.08	120.30

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	2	105	ARG	Peptide
1	2	183	LYS	Peptide
1	5	171	ARG	Peptide
1	6	110	MET	Peptide
1	6	172	MET	Peptide
1	7	116	VAL	Peptide
1	O	155	GLU	Peptide

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	808	0	817	47	0
1	2	773	0	784	43	0
1	3	762	0	775	52	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	4	762	0	775	47	0
1	5	762	0	775	64	0
1	6	773	0	784	75	0
1	7	808	0	817	56	0
1	A	808	0	817	20	0
1	B	808	0	817	27	0
1	C	808	0	817	33	0
1	D	773	0	784	20	0
1	E	808	0	817	30	0
1	F	808	0	817	38	0
1	G	808	0	817	47	0
1	H	782	0	790	37	0
1	I	808	0	817	39	1
1	J	791	0	798	25	0
1	K	808	0	817	41	0
1	L	808	0	817	28	1
1	M	808	0	817	43	0
1	N	782	0	790	59	0
1	O	808	0	817	50	0
1	P	762	0	775	68	0
1	Q	808	0	817	35	0
1	R	808	0	817	24	1
1	T	808	0	817	22	0
1	U	791	0	798	24	0
1	V	808	0	817	32	0
1	W	808	0	817	37	0
1	X	808	0	817	28	0
1	Y	808	0	817	34	1
1	Z	762	0	775	53	0
2	1	8	0	0	3	0
2	2	7	0	0	0	0
2	3	18	0	0	2	0
2	4	6	0	0	0	0
2	5	14	0	0	2	0
2	6	3	0	0	0	0
2	7	9	0	0	2	0
2	A	21	0	0	4	0
2	B	24	0	0	4	0
2	C	25	0	0	4	0
2	D	39	0	0	2	0
2	E	21	0	0	2	0
2	F	30	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	G	19	0	0	4	0
2	H	26	0	0	1	0
2	I	3	0	0	0	0
2	J	10	0	0	0	0
2	K	5	0	0	0	0
2	L	17	0	0	2	0
2	M	5	0	0	1	0
2	N	13	0	0	5	0
2	O	3	0	0	1	0
2	P	8	0	0	3	0
2	Q	18	0	0	2	0
2	R	33	0	0	2	0
2	T	32	0	0	4	0
2	U	27	0	0	2	0
2	V	16	0	0	2	0
2	W	27	0	0	4	0
2	X	19	0	0	3	0
2	Y	17	0	0	5	0
2	Z	4	0	0	2	0
All	All	25962	0	25743	1083	2

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 21.

All (1083) 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:P:111:THR:O	1:P:115:LYS:HE2	1.42	1.18
1:P:109:GLU:CD	1:P:115:LYS:HZ2	1.54	1.09
1:P:111:THR:O	1:P:115:LYS:CE	2.00	1.09
1:6:94:LYS:HD3	1:6:132:LYS:O	1.53	1.09
1:M:114:LYS:NZ	2:M:201:HOH:O	1.89	1.06
1:6:156:MET:O	1:6:156:MET:HG3	1.54	1.04
1:5:169:ASP:O	1:5:173:TYR:OH	1.76	1.04
1:P:109:GLU:CD	1:P:115:LYS:NZ	2.11	1.03
1:7:170:HIS:CD2	1:7:173:TYR:HE2	1.81	0.98
1:P:109:GLU:OE1	1:P:115:LYS:NZ	1.98	0.96
1:M:176:LEU:HD23	1:M:177:PRO:O	1.64	0.96
1:W:173:TYR:CZ	1:W:181:LYS:HE2	2.03	0.93
1:2:158:ILE:HD11	1:2:165:ILE:HD13	1.50	0.93
1:I:185:THR:O	1:I:188:ILE:HG23	1.67	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:187:PHE:HA	1:Q:190:PHE:CD2	2.04	0.93
1:E:92:VAL:N	2:E:201:HOH:O	2.03	0.92
1:E:131:MET:O	1:H:171:ARG:NH2	2.03	0.92
1:C:176:LEU:HB3	1:C:180:GLU:OE2	1.68	0.91
1:Z:171:ARG:HG3	1:1:164:GLY:HA2	1.51	0.90
1:P:120:ALA:HB1	1:P:122:ILE:HG12	1.51	0.89
1:7:170:HIS:CD2	1:7:173:TYR:CE2	2.60	0.89
1:B:103:TRP:O	1:B:106:LYS:O	1.90	0.89
1:P:109:GLU:OE2	1:P:115:LYS:NZ	2.03	0.88
1:Y:107:ASP:O	1:Y:110:MET:HB2	1.72	0.88
1:3:171:ARG:O	1:3:173:TYR:N	2.08	0.87
1:B:181:LYS:NZ	2:B:201:HOH:O	2.06	0.87
1:T:105:ARG:NH1	2:T:201:HOH:O	2.07	0.86
1:3:142:LEU:HD21	1:3:157:ILE:HD11	1.57	0.85
1:W:173:TYR:CE2	1:W:181:LYS:HE2	2.11	0.85
1:1:146:ALA:HB1	1:1:152:GLU:HA	1.58	0.85
1:P:123:GLY:O	1:P:126:THR:O	1.95	0.85
1:N:178:GLN:HB2	1:N:181:LYS:HB3	1.58	0.84
1:M:139:ILE:HD11	1:N:93:GLU:HG3	1.60	0.83
1:O:173:TYR:HB2	1:O:176:LEU:HD11	1.60	0.83
1:U:191:VAL:O	1:U:193:GLU:HA	1.77	0.83
1:K:154:TYR:HE1	1:L:157:ILE:C	1.83	0.82
1:I:189:ASN:O	1:I:191:VAL:N	2.12	0.81
1:4:170:HIS:CE1	1:5:164:GLY:O	2.33	0.81
1:7:162:ALA:HB1	1:7:163:PRO:HA	1.62	0.81
1:Z:176:LEU:HG	1:Z:177:PRO:HD2	1.62	0.81
1:Q:92:VAL:N	2:Q:201:HOH:O	2.12	0.81
1:Z:170:HIS:HB3	1:Z:172:MET:N	1.95	0.81
1:6:169:ASP:OD1	1:6:172:MET:HA	1.82	0.79
1:A:138:THR:OG1	1:B:136:SER:O	2.00	0.79
1:6:170:HIS:CD2	1:7:164:GLY:O	2.36	0.79
1:T:110:MET:HG2	1:T:115:LYS:HB3	1.62	0.79
1:3:173:TYR:O	1:3:181:LYS:HE2	1.83	0.79
1:4:96:ALA:O	1:4:99:THR:HG22	1.83	0.78
1:N:182:ASN:HB3	1:N:186:SER:HB3	1.64	0.78
1:O:190:PHE:CE1	1:O:191:VAL:HB	2.18	0.78
1:R:113:GLU:OE1	1:R:128:ASN:ND2	2.17	0.78
1:6:129:ARG:CD	1:6:132:LYS:HE2	2.11	0.78
1:O:194:GLN:NE2	1:P:172:MET:O	2.16	0.78
1:H:187:PHE:O	1:H:190:PHE:HD2	1.66	0.78
1:2:109:GLU:HG3	1:2:149:PHE:HE1	1.48	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:193:GLU:HA	1:I:196:LYS:HB3	1.66	0.77
1:K:116:VAL:O	1:K:127:VAL:HG11	1.85	0.77
1:N:143:SER:HA	1:N:153:ALA:HB2	1.66	0.77
1:D:92:VAL:N	2:D:202:HOH:O	2.16	0.77
1:P:190:PHE:O	1:P:191:VAL:HG22	1.83	0.77
1:F:193:GLU:O	1:F:196:LYS:NZ	2.12	0.77
1:O:171:ARG:CZ	1:O:174:ALA:HB1	2.14	0.77
1:N:181:LYS:HG2	1:N:182:ASN:N	1.97	0.76
1:7:97:ALA:HB2	1:7:133:ALA:HB2	1.65	0.76
1:N:173:TYR:CE2	1:N:183:LYS:HG3	2.21	0.76
1:M:155:GLU:OE2	1:M:170:HIS:ND1	2.18	0.76
1:Q:190:PHE:CE2	1:1:190:PHE:CE1	2.73	0.76
1:6:129:ARG:HD3	1:6:132:LYS:HE2	1.65	0.76
1:6:104:MET:CE	1:6:111:THR:O	2.34	0.76
1:E:136:SER:HB3	1:F:138:THR:HG23	1.66	0.76
1:2:96:ALA:HB1	1:2:100:LEU:HD23	1.67	0.75
1:M:155:GLU:CD	1:M:170:HIS:HD1	1.89	0.75
1:Z:189:ASN:OD1	1:Z:190:PHE:CD2	2.38	0.75
1:Z:170:HIS:HB3	1:Z:171:ARG:C	2.06	0.75
1:H:187:PHE:O	1:H:190:PHE:CD2	2.40	0.75
1:6:104:MET:HE3	1:6:111:THR:O	1.87	0.75
1:Q:150:GLY:O	1:Q:171:ARG:HD3	1.86	0.74
1:7:112:SER:O	1:7:115:LYS:HE2	1.86	0.74
1:P:117:ALA:O	1:P:121:GLY:N	2.19	0.74
1:F:171:ARG:HE	1:G:132:LYS:HG3	1.53	0.74
1:4:93:GLU:O	1:4:97:ALA:N	2.20	0.73
1:A:156:MET:HE3	2:A:208:HOH:O	1.86	0.73
1:A:169:ASP:OD1	1:A:171:ARG:HG2	1.88	0.73
1:O:173:TYR:CE2	1:P:191:VAL:HG23	2.23	0.73
1:D:108:THR:OG1	2:D:201:HOH:O	2.06	0.73
1:O:108:THR:O	1:O:109:GLU:HB3	1.89	0.73
1:I:116:VAL:HG21	1:I:127:VAL:HG21	1.70	0.73
1:P:176:LEU:HA	1:P:177:PRO:C	2.09	0.73
1:2:110:MET:HG3	1:2:149:PHE:CZ	2.24	0.72
1:4:136:SER:OG	1:5:140:GLY:N	2.22	0.72
1:T:173:TYR:O	1:T:181:LYS:NZ	2.21	0.72
1:5:171:ARG:HG2	1:5:172:MET:N	2.03	0.72
1:6:111:THR:HG23	1:6:112:SER:H	1.55	0.72
1:I:157:ILE:HD11	1:J:154:TYR:N	2.04	0.72
1:M:155:GLU:OE2	1:M:170:HIS:CE1	2.42	0.72
1:6:99:THR:N	1:6:156:MET:HE1	2.04	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:129:ARG:NH2	2:U:201:HOH:O	2.22	0.72
1:5:97:ALA:HB2	1:5:133:ALA:HB2	1.72	0.72
1:E:157:ILE:HD11	1:F:157:ILE:HD11	1.71	0.72
1:W:143:SER:O	1:W:147:ARG:HG2	1.89	0.71
1:N:176:LEU:HD22	1:N:178:GLN:HE21	1.54	0.71
1:E:131:MET:O	1:H:171:ARG:CZ	2.38	0.71
1:6:154:TYR:CE2	1:6:170:HIS:HB3	2.25	0.71
1:T:92:VAL:HG12	2:T:220:HOH:O	1.90	0.71
1:Z:153:ALA:HA	2:Z:201:HOH:O	1.90	0.70
1:Q:109:GLU:HG3	1:Q:110:MET:HG3	1.73	0.70
1:P:111:THR:C	1:P:115:LYS:CE	2.60	0.70
1:N:182:ASN:HB3	1:N:186:SER:CB	2.21	0.70
1:K:99:THR:HG21	1:K:158:ILE:HD13	1.74	0.70
1:M:176:LEU:CD2	1:M:177:PRO:O	2.39	0.70
1:N:192:PHE:O	1:N:193:GLU:HB2	1.91	0.70
1:6:169:ASP:O	1:6:170:HIS:HB2	1.91	0.69
1:6:95:GLN:HG2	1:6:156:MET:HG2	1.74	0.69
1:P:117:ALA:HB2	1:P:127:VAL:HG22	1.74	0.69
1:I:174:ALA:O	1:I:178:GLN:NE2	2.25	0.69
1:P:190:PHE:O	1:P:191:VAL:CG2	2.40	0.69
1:O:153:ALA:HB3	1:P:159:PRO:HD3	1.74	0.69
1:U:178:GLN:O	1:U:182:ASN:ND2	2.26	0.69
1:G:111:THR:HG21	1:G:115:LYS:N	2.07	0.69
1:Z:128:ASN:O	1:Z:131:MET:HB3	1.93	0.69
1:J:158:ILE:HD11	1:J:165:ILE:HG21	1.73	0.69
1:6:156:MET:O	1:6:156:MET:CG	2.35	0.69
1:P:111:THR:N	1:P:115:LYS:HZ3	1.91	0.69
1:A:173:TYR:O	1:A:181:LYS:NZ	2.25	0.68
1:7:116:VAL:HA	1:7:118:VAL:HG12	1.75	0.68
1:K:113:GLU:OE1	1:K:130:ILE:N	2.26	0.68
1:N:182:ASN:CB	1:N:186:SER:HB3	2.24	0.68
1:U:147:ARG:NH1	1:U:152:GLU:OE2	2.26	0.68
1:Z:169:ASP:O	1:Z:171:ARG:HA	1.94	0.67
1:6:95:GLN:O	1:6:156:MET:HE3	1.95	0.67
1:5:114:LYS:HG2	1:5:128:ASN:OD1	1.94	0.67
1:V:166:ILE:HG12	1:W:173:TYR:CZ	2.29	0.67
1:Y:104:MET:O	1:Y:110:MET:HA	1.94	0.67
1:6:169:ASP:OD1	1:6:172:MET:CA	2.42	0.67
1:O:157:ILE:HD12	1:P:154:TYR:HA	1.77	0.67
1:T:149:PHE:O	1:T:171:ARG:NH2	2.27	0.67
1:5:156:MET:SD	2:5:209:HOH:O	2.53	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:6:109:GLU:O	1:6:111:THR:HG22	1.95	0.66
1:B:94:LYS:HD2	1:B:94:LYS:H	1.59	0.66
1:2:168:TYR:CE2	1:3:166:ILE:HD11	2.30	0.66
1:V:166:ILE:HA	1:W:173:TYR:OH	1.95	0.66
1:G:110:MET:CE	1:G:116:VAL:HG23	2.25	0.66
1:L:116:VAL:O	1:L:120:ALA:O	2.13	0.66
1:Q:142:LEU:HG	1:Q:156:MET:HE3	1.77	0.66
1:Q:107:ASP:OD1	1:Q:108:THR:N	2.29	0.66
1:2:158:ILE:HD12	1:2:159:PRO:HD2	1.78	0.65
1:O:173:TYR:CB	1:O:176:LEU:HD11	2.26	0.65
1:K:154:TYR:CE1	1:L:157:ILE:C	2.70	0.65
1:V:97:ALA:HB2	1:V:133:ALA:HB2	1.78	0.65
1:I:150:GLY:O	1:I:171:ARG:NE	2.29	0.65
1:O:139:ILE:HG22	1:P:139:ILE:HD13	1.77	0.65
1:P:169:ASP:OD1	1:P:171:ARG:HB2	1.95	0.65
1:V:110:MET:HE1	1:V:115:LYS:HG2	1.78	0.65
1:V:189:ASN:O	1:V:193:GLU:OE1	2.13	0.65
1:W:122:ILE:HG12	1:W:126:THR:OG1	1.97	0.65
1:N:182:ASN:HA	1:N:185:THR:HB	1.78	0.65
1:6:93:GLU:C	1:6:133:ALA:HB2	2.17	0.65
1:P:103:TRP:O	1:P:106:LYS:HG2	1.96	0.65
1:W:130:ILE:HG12	1:W:137:THR:OG1	1.96	0.64
1:L:128:ASN:OD1	1:L:132:LYS:NZ	2.30	0.64
1:P:111:THR:O	1:P:115:LYS:HE3	1.92	0.64
1:Y:189:ASN:OD1	1:Y:190:PHE:N	2.30	0.64
1:Z:125:ALA:C	1:Z:127:VAL:HG22	2.17	0.64
1:Z:171:ARG:HB3	1:Z:173:TYR:HB3	1.79	0.64
1:T:122:ILE:HD13	1:T:141:VAL:HG13	1.80	0.64
1:A:138:THR:HA	1:B:138:THR:HA	1.78	0.64
1:6:146:ALA:HB1	1:6:151:HIS:O	1.98	0.64
1:G:128:ASN:ND2	2:G:201:HOH:O	2.30	0.64
1:2:126:THR:O	1:2:130:ILE:HG13	1.97	0.64
1:5:171:ARG:HG2	1:5:172:MET:H	1.62	0.63
1:X:178:GLN:O	2:X:201:HOH:O	2.15	0.63
1:6:168:TYR:CZ	1:6:170:HIS:CD2	2.85	0.63
1:7:103:TRP:HB3	1:7:149:PHE:CZ	2.33	0.63
1:X:108:THR:N	1:X:109:GLU:HA	2.13	0.63
1:Z:189:ASN:OD1	1:Z:190:PHE:CG	2.51	0.63
1:1:186:SER:HA	1:1:189:ASN:HB2	1.80	0.63
1:I:159:PRO:HD3	1:J:154:TYR:CE1	2.34	0.63
1:K:103:TRP:HE1	1:K:158:ILE:HD11	1.64	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:155:GLU:CD	1:M:170:HIS:ND1	2.51	0.63
1:N:95:GLN:NE2	2:N:202:HOH:O	2.31	0.63
1:O:107:ASP:O	1:O:109:GLU:N	2.32	0.63
1:I:126:THR:O	1:I:130:ILE:N	2.24	0.63
1:Q:142:LEU:O	1:Q:156:MET:HE1	1.98	0.63
1:F:171:ARG:O	1:F:171:ARG:NH1	2.32	0.63
1:Q:105:ARG:NH1	1:U:175:ALA:O	2.32	0.63
1:V:166:ILE:HG12	1:W:173:TYR:CE2	2.34	0.63
1:7:103:TRP:HB3	1:7:149:PHE:HZ	1.64	0.63
1:D:158:ILE:O	1:F:105:ARG:NH2	2.32	0.63
1:G:110:MET:HE2	1:G:116:VAL:HA	1.80	0.63
1:I:190:PHE:CE1	1:J:184:ILE:HD11	2.34	0.63
1:5:97:ALA:CB	1:5:133:ALA:HB2	2.29	0.62
1:U:179:GLU:HG3	1:3:179:GLU:CD	2.18	0.62
1:4:92:VAL:N	1:4:95:GLN:OE1	2.32	0.62
1:N:171:ARG:HG2	1:N:172:MET:N	2.15	0.62
1:W:173:TYR:CZ	1:W:181:LYS:CE	2.81	0.62
1:W:135:VAL:N	2:W:201:HOH:O	2.31	0.62
1:6:99:THR:H	1:6:156:MET:HE1	1.63	0.62
1:I:189:ASN:C	1:I:191:VAL:H	2.02	0.62
1:X:110:MET:HG3	1:X:111:THR:N	2.14	0.62
1:O:176:LEU:HD13	1:O:180:GLU:CD	2.20	0.62
1:1:142:LEU:HD13	1:1:153:ALA:HB2	1.82	0.62
1:G:111:THR:HG21	1:G:116:VAL:N	2.14	0.62
1:R:104:MET:SD	1:R:112:SER:N	2.72	0.62
1:O:190:PHE:CE1	1:Y:189:ASN:ND2	2.68	0.62
1:N:117:ALA:HB2	1:N:127:VAL:HG11	1.81	0.61
1:N:178:GLN:OE1	1:N:181:LYS:CB	2.47	0.61
1:B:106:LYS:O	1:B:107:ASP:CB	2.48	0.61
1:1:162:ALA:HB3	1:7:132:LYS:NZ	2.15	0.61
1:3:178:GLN:HA	1:3:181:LYS:HE3	1.83	0.61
1:L:116:VAL:HG11	1:L:127:VAL:HG21	1.82	0.61
1:4:158:ILE:HG12	1:4:165:ILE:HG21	1.82	0.61
1:C:106:LYS:O	1:C:110:MET:SD	2.58	0.61
1:I:191:VAL:HB	1:I:195:ASN:HB2	1.83	0.61
1:P:109:GLU:O	1:P:110:MET:HB2	2.00	0.61
1:5:117:ALA:HB2	1:5:127:VAL:HG21	1.83	0.61
1:T:127:VAL:O	1:T:131:MET:HG3	2.01	0.61
1:7:109:GLU:OE2	1:7:149:PHE:HA	2.01	0.61
1:P:111:THR:C	1:P:115:LYS:HE3	2.21	0.61
1:O:168:TYR:OH	1:P:164:GLY:O	2.17	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:99:THR:HG23	1:7:102:ALA:HB2	1.82	0.60
1:P:110:MET:C	1:P:115:LYS:HZ3	2.04	0.60
1:6:191:VAL:HG12	1:6:191:VAL:O	2.02	0.60
1:5:170:HIS:O	1:5:173:TYR:CE2	2.53	0.60
1:P:126:THR:HG22	1:P:128:ASN:H	1.65	0.60
1:5:170:HIS:C	1:5:173:TYR:CE2	2.74	0.60
1:3:93:GLU:HG2	1:3:136:SER:HA	1.84	0.60
1:6:111:THR:HG23	1:6:112:SER:N	2.17	0.60
1:6:95:GLN:O	1:6:156:MET:CE	2.50	0.60
1:C:117:ALA:HB2	1:C:127:VAL:HG11	1.83	0.60
1:J:142:LEU:HD13	1:J:153:ALA:HB1	1.84	0.60
1:J:172:MET:HG3	1:J:175:ALA:HB3	1.84	0.60
1:R:113:GLU:HB3	1:R:128:ASN:OD1	2.02	0.60
1:3:138:THR:HG22	1:3:141:VAL:HG22	1.83	0.60
1:O:190:PHE:HB2	1:Y:190:PHE:HA	1.84	0.60
1:2:126:THR:HA	1:2:129:ARG:HB2	1.83	0.60
1:H:188:ILE:O	1:H:191:VAL:N	2.34	0.60
1:M:182:ASN:HA	1:M:185:THR:HB	1.83	0.60
1:L:114:LYS:HA	1:L:124:PRO:HB3	1.83	0.59
1:Y:173:TYR:HA	1:Y:176:LEU:HD22	1.82	0.59
1:L:115:LYS:NZ	2:L:201:HOH:O	2.35	0.59
1:5:171:ARG:HG2	1:5:173:TYR:N	2.16	0.59
1:F:138:THR:HG22	1:F:140:GLY:H	1.67	0.59
1:I:189:ASN:O	1:I:190:PHE:CD1	2.56	0.59
1:I:134:GLU:O	1:I:135:VAL:HG13	2.02	0.59
1:Y:94:LYS:HD2	1:Y:94:LYS:H	1.67	0.59
1:B:104:MET:HB3	1:B:111:THR:HG23	1.82	0.59
1:U:130:ILE:HG12	1:U:137:THR:OG1	2.03	0.59
1:O:139:ILE:HD11	1:P:93:GLU:HB3	1.83	0.59
1:6:129:ARG:HD2	1:6:132:LYS:HE2	1.85	0.59
1:A:166:ILE:HG12	1:B:173:TYR:CZ	2.37	0.59
1:L:129:ARG:O	1:L:133:ALA:N	2.36	0.59
1:2:100:LEU:HD11	1:2:131:MET:HA	1.85	0.58
1:Q:142:LEU:HG	1:Q:156:MET:CE	2.33	0.58
1:H:190:PHE:CD1	1:H:191:VAL:N	2.71	0.58
1:A:142:LEU:HD12	2:A:208:HOH:O	2.03	0.58
1:Z:158:ILE:N	1:1:154:TYR:OH	2.36	0.58
1:5:170:HIS:O	1:5:170:HIS:CD2	2.56	0.58
1:5:171:ARG:HG3	1:5:174:ALA:H	1.68	0.58
1:5:143:SER:O	1:5:147:ARG:HG3	2.03	0.58
1:5:188:ILE:O	1:5:191:VAL:HG22	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:126:THR:HG23	1:J:129:ARG:CZ	2.34	0.58
1:O:185:THR:HG22	1:P:166:ILE:HG23	1.86	0.58
1:L:189:ASN:O	1:L:192:PHE:CD1	2.57	0.58
1:U:185:THR:O	1:U:189:ASN:ND2	2.32	0.58
1:3:142:LEU:HD21	1:3:157:ILE:CD1	2.33	0.58
1:O:108:THR:O	1:O:109:GLU:CB	2.51	0.58
1:G:158:ILE:HG22	1:H:154:TYR:CG	2.39	0.58
1:M:157:ILE:HG13	1:M:157:ILE:O	2.03	0.58
1:X:110:MET:SD	1:X:111:THR:OG1	2.61	0.58
1:W:173:TYR:CE2	1:W:181:LYS:CE	2.87	0.58
1:6:132:LYS:O	1:6:133:ALA:HB3	2.04	0.57
1:N:181:LYS:CG	1:N:182:ASN:N	2.67	0.57
1:N:182:ASN:HB2	1:W:183:LYS:NZ	2.19	0.57
1:O:99:THR:OG1	1:O:156:MET:HG3	2.04	0.57
1:W:191:VAL:O	1:W:195:ASN:ND2	2.36	0.57
1:P:109:GLU:OE2	1:P:115:LYS:CD	2.52	0.57
1:T:93:GLU:CD	1:T:93:GLU:H	2.08	0.57
1:7:187:PHE:HA	1:7:190:PHE:CE2	2.39	0.57
1:Z:158:ILE:HD12	1:1:154:TYR:CZ	2.40	0.57
1:1:129:ARG:O	1:1:133:ALA:O	2.22	0.57
1:4:154:TYR:CE2	1:5:158:ILE:HD13	2.39	0.57
1:6:171:ARG:O	1:6:174:ALA:N	2.37	0.57
1:H:92:VAL:HG13	1:H:93:GLU:H	1.70	0.57
1:T:129:ARG:NH2	2:T:202:HOH:O	2.36	0.57
1:2:104:MET:HG3	1:2:105:ARG:N	2.20	0.57
1:4:99:THR:HG21	1:4:156:MET:CA	2.35	0.57
1:A:168:TYR:OH	1:B:164:GLY:O	2.14	0.57
1:K:190:PHE:O	1:K:193:GLU:HG3	2.05	0.57
1:3:114:LYS:HE3	1:3:124:PRO:HB2	1.85	0.57
1:5:171:ARG:HG3	1:5:174:ALA:N	2.20	0.57
1:X:166:ILE:HG22	1:Y:173:TYR:CZ	2.40	0.57
1:4:170:HIS:ND1	1:5:164:GLY:O	2.37	0.57
1:E:131:MET:O	1:H:171:ARG:NH1	2.38	0.57
1:P:111:THR:N	1:P:115:LYS:NZ	2.52	0.57
1:X:151:HIS:ND1	1:X:155:GLU:OE1	2.33	0.57
1:F:113:GLU:HG2	1:F:131:MET:SD	2.45	0.56
1:N:178:GLN:OE1	1:N:181:LYS:HB2	2.05	0.56
1:V:110:MET:SD	1:V:115:LYS:HG2	2.44	0.56
1:Z:128:ASN:OD1	1:Z:131:MET:SD	2.63	0.56
1:2:122:ILE:HD11	1:2:145:LEU:CD2	2.35	0.56
1:3:137:THR:HG22	1:3:141:VAL:HG23	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:151:HIS:HE2	1:7:106:LYS:HG2	1.70	0.56
1:P:117:ALA:HB2	1:P:127:VAL:CG2	2.35	0.56
1:W:193:GLU:HA	1:W:196:LYS:HG2	1.87	0.56
1:F:130:ILE:HG12	1:F:137:THR:CG2	2.35	0.56
1:G:111:THR:HG21	1:G:116:VAL:H	1.71	0.56
1:N:100:LEU:HD13	1:N:145:LEU:HD21	1.85	0.56
1:M:192:PHE:HZ	1:W:186:SER:CB	2.18	0.56
1:X:143:SER:HB2	1:Y:92:VAL:HG21	1.87	0.56
1:6:94:LYS:N	1:6:133:ALA:HB2	2.19	0.56
1:H:189:ASN:HA	1:H:191:VAL:HG23	1.86	0.56
1:K:173:TYR:O	1:K:181:LYS:NZ	2.39	0.56
1:M:97:ALA:HA	1:M:131:MET:HB3	1.87	0.56
1:M:94:LYS:HA	1:M:132:LYS:HA	1.87	0.56
1:N:94:LYS:H	1:N:94:LYS:HD2	1.69	0.56
1:6:187:PHE:HE2	1:7:183:LYS:HE2	1.70	0.56
1:A:93:GLU:OE2	1:A:136:SER:OG	2.24	0.56
1:Q:187:PHE:HE2	1:R:184:ILE:HA	1.71	0.56
1:O:139:ILE:HG23	1:P:137:THR:O	2.06	0.56
1:O:190:PHE:CD1	1:O:191:VAL:HB	2.40	0.56
1:Q:176:LEU:HD21	1:R:192:PHE:HA	1.87	0.56
1:Q:190:PHE:CE2	1:1:190:PHE:CD1	2.94	0.56
1:W:105:ARG:HG2	1:W:105:ARG:HH11	1.70	0.56
1:J:187:PHE:O	1:J:190:PHE:HB3	2.06	0.56
1:O:127:VAL:O	1:O:130:ILE:HG22	2.05	0.56
1:1:169:ASP:HB3	1:1:172:MET:HG2	1.88	0.56
1:I:114:LYS:O	1:I:115:LYS:O	2.22	0.56
1:O:174:ALA:O	1:O:181:LYS:NZ	2.39	0.56
1:Q:188:ILE:HG22	1:Q:192:PHE:CE2	2.40	0.56
1:2:143:SER:O	1:2:147:ARG:HG2	2.05	0.56
1:N:171:ARG:CG	1:N:172:MET:N	2.69	0.56
1:M:184:ILE:HG21	1:N:188:ILE:HD11	1.88	0.56
1:N:92:VAL:N	2:N:203:HOH:O	2.38	0.56
1:D:191:VAL:HG12	1:D:191:VAL:O	2.07	0.55
1:K:158:ILE:HD12	1:K:158:ILE:N	2.21	0.55
1:U:183:LYS:O	1:U:186:SER:OG	2.21	0.55
1:2:100:LEU:HD22	1:2:130:ILE:HG22	1.87	0.55
1:K:154:TYR:CE1	1:L:157:ILE:HB	2.40	0.55
1:2:136:SER:C	1:3:138:THR:OG1	2.44	0.55
1:K:154:TYR:CE1	1:L:157:ILE:O	2.60	0.55
1:O:171:ARG:NH1	1:O:174:ALA:HB1	2.21	0.55
1:Q:147:ARG:NH1	1:Q:152:GLU:OE2	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:99:THR:HG21	1:3:156:MET:HA	1.88	0.55
1:G:95:GLN:NE2	1:G:158:ILE:O	2.40	0.55
1:6:99:THR:HG22	1:6:103:TRP:NE1	2.22	0.55
1:R:179:GLU:HA	1:R:182:ASN:HB2	1.88	0.55
1:4:187:PHE:CE2	1:5:187:PHE:HB3	2.42	0.55
1:7:170:HIS:C	1:7:170:HIS:CD2	2.80	0.55
1:1:129:ARG:HB3	1:1:135:VAL:HG11	1.88	0.55
1:6:100:LEU:HA	1:6:103:TRP:CE3	2.41	0.55
1:K:160:VAL:HG22	1:K:161:GLY:H	1.71	0.55
1:M:178:GLN:HB2	1:M:182:ASN:OD1	2.06	0.55
1:Z:138:THR:HA	1:1:138:THR:HA	1.89	0.55
1:7:110:MET:O	1:7:115:LYS:NZ	2.22	0.55
1:6:129:ARG:HD3	1:6:132:LYS:CE	2.36	0.54
1:N:92:VAL:O	2:N:201:HOH:O	2.18	0.54
1:7:169:ASP:OD1	1:7:170:HIS:N	2.40	0.54
1:C:177:PRO:O	1:C:180:GLU:OE2	2.25	0.54
1:M:96:ALA:HA	1:M:156:MET:O	2.07	0.54
1:O:139:ILE:N	1:P:137:THR:O	2.35	0.54
1:4:99:THR:HG21	1:4:156:MET:HA	1.90	0.54
1:5:97:ALA:HB2	1:5:133:ALA:CB	2.36	0.54
1:G:108:THR:N	1:G:109:GLU:HA	2.23	0.54
1:G:111:THR:CG2	1:G:116:VAL:N	2.71	0.54
1:K:152:GLU:O	1:K:154:TYR:N	2.40	0.54
1:U:162:ALA:HB2	1:W:105:ARG:NH2	2.23	0.54
1:C:110:MET:HB2	1:C:115:LYS:HE3	1.88	0.54
1:C:195:ASN:HD22	1:C:195:ASN:N	2.05	0.54
1:2:110:MET:O	1:2:115:LYS:HD3	2.07	0.54
1:6:94:LYS:HA	1:6:132:LYS:O	2.07	0.54
1:7:103:TRP:CE3	1:7:149:PHE:CE1	2.96	0.54
1:2:136:SER:HA	1:3:139:ILE:HG13	1.90	0.54
1:4:110:MET:SD	1:4:115:LYS:HG2	2.47	0.54
1:C:105:ARG:NH2	2:C:201:HOH:O	2.22	0.54
1:O:157:ILE:HD13	1:P:157:ILE:HD11	1.90	0.54
1:G:144:SER:HA	1:G:147:ARG:NH1	2.22	0.54
1:H:112:SER:OG	1:H:114:LYS:HB3	2.07	0.54
1:I:116:VAL:HG21	1:I:127:VAL:CG2	2.38	0.54
1:5:152:GLU:HB2	1:5:154:TYR:CE2	2.43	0.54
1:G:111:THR:HG23	1:G:116:VAL:HG12	1.88	0.54
1:C:114:LYS:HA	1:C:117:ALA:HB3	1.89	0.54
1:H:173:TYR:CE1	1:H:184:ILE:HD11	2.43	0.53
1:W:101:ASN:HD21	1:W:105:ARG:NH2	2.06	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:104:MET:SD	1:1:131:MET:SD	3.07	0.53
1:4:134:GLU:HG3	1:4:135:VAL:HG23	1.91	0.53
1:T:147:ARG:NH1	2:T:203:HOH:O	2.39	0.53
1:D:117:ALA:HB2	1:D:127:VAL:HG21	1.91	0.53
1:H:190:PHE:CG	1:H:191:VAL:N	2.76	0.53
1:O:110:MET:SD	1:O:149:PHE:CE1	3.02	0.53
1:W:193:GLU:O	1:W:196:LYS:HG3	2.08	0.53
1:Y:101:ASN:OD1	1:Y:131:MET:HG3	2.09	0.53
1:P:180:GLU:N	1:Y:179:GLU:HG2	2.24	0.53
1:5:171:ARG:HG2	1:5:173:TYR:H	1.74	0.53
1:7:190:PHE:HA	1:7:193:GLU:OE2	2.08	0.53
1:L:189:ASN:O	1:L:192:PHE:HD1	1.91	0.53
1:N:182:ASN:HB3	1:N:186:SER:N	2.24	0.53
1:K:136:SER:HB3	1:L:138:THR:HG21	1.89	0.53
1:V:110:MET:CG	1:V:116:VAL:HG13	2.38	0.53
1:X:143:SER:O	1:X:147:ARG:HB2	2.09	0.53
1:3:146:ALA:HB1	1:3:151:HIS:O	2.08	0.53
1:B:106:LYS:O	1:B:107:ASP:HB3	2.07	0.53
1:G:114:LYS:C	1:G:116:VAL:H	2.11	0.53
1:O:172:MET:HE1	2:O:203:HOH:O	2.08	0.53
1:4:99:THR:HG21	1:4:156:MET:CB	2.38	0.53
1:6:169:ASP:OD1	1:6:172:MET:N	2.40	0.53
1:6:157:ILE:HG23	1:7:154:TYR:CB	2.39	0.53
1:1:94:LYS:H	1:1:94:LYS:HD2	1.72	0.53
1:4:187:PHE:HE2	1:5:184:ILE:HA	1.73	0.53
1:F:196:LYS:NZ	2:F:202:HOH:O	2.39	0.53
1:Z:184:ILE:HA	1:Z:187:PHE:CZ	2.44	0.53
1:N:165:ILE:HG22	1:N:166:ILE:N	2.24	0.53
1:P:120:ALA:CB	1:P:122:ILE:HG12	2.32	0.53
1:V:116:VAL:HG21	1:V:127:VAL:HG11	1.90	0.53
1:N:182:ASN:HB2	1:W:183:LYS:HZ1	1.74	0.53
1:C:168:TYR:CZ	1:D:166:ILE:HD12	2.43	0.52
1:P:109:GLU:OE2	1:P:115:LYS:CE	2.57	0.52
1:6:184:ILE:HD11	1:7:188:ILE:HG23	1.90	0.52
1:M:157:ILE:HD11	1:N:154:TYR:HB3	1.91	0.52
1:6:132:LYS:HZ2	1:6:132:LYS:H	1.57	0.52
1:E:103:TRP:CH2	1:E:151:HIS:HB2	2.45	0.52
1:6:100:LEU:O	1:6:104:MET:HG2	2.09	0.52
1:6:187:PHE:CE2	1:7:183:LYS:HE2	2.45	0.52
1:F:138:THR:HG22	1:F:140:GLY:N	2.25	0.52
1:L:180:GLU:HG2	2:L:213:HOH:O	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:92:VAL:HG23	1:L:93:GLU:HG3	1.91	0.52
1:P:109:GLU:OE2	1:P:115:LYS:HD2	2.10	0.52
1:Q:178:GLN:HA	1:Q:181:LYS:HG3	1.92	0.52
1:Z:158:ILE:HD12	1:1:154:TYR:CE2	2.44	0.52
1:2:122:ILE:HD11	1:2:145:LEU:HD22	1.90	0.52
1:N:178:GLN:OE1	1:N:181:LYS:HD2	2.09	0.52
1:P:100:LEU:HD13	1:P:156:MET:HE3	1.92	0.52
1:V:109:GLU:N	1:V:109:GLU:OE1	2.42	0.52
1:1:162:ALA:HB3	1:7:132:LYS:HZ3	1.74	0.52
1:C:173:TYR:CZ	1:D:166:ILE:HG13	2.44	0.52
1:H:188:ILE:O	1:H:191:VAL:CG2	2.57	0.52
1:X:110:MET:O	1:X:111:THR:HG23	2.10	0.52
1:2:188:ILE:O	1:2:191:VAL:HG12	2.09	0.52
1:6:176:LEU:HG	1:6:180:GLU:CG	2.39	0.52
1:I:178:GLN:HG3	1:I:181:LYS:HD2	1.92	0.52
1:P:162:ALA:HB3	1:P:165:ILE:CG2	2.40	0.52
1:R:105:ARG:HD2	1:R:111:THR:HG21	1.91	0.52
1:C:182:ASN:O	1:C:186:SER:N	2.41	0.52
1:E:162:ALA:HB3	1:E:165:ILE:HD12	1.91	0.52
1:K:120:ALA:HB2	1:K:127:VAL:CG1	2.40	0.52
1:V:92:VAL:N	2:V:201:HOH:O	2.41	0.52
1:X:166:ILE:HG22	1:Y:173:TYR:CE1	2.44	0.52
1:Z:151:HIS:CD2	1:Z:170:HIS:O	2.62	0.52
1:6:176:LEU:HG	1:6:180:GLU:HG2	1.91	0.52
1:G:102:ALA:HA	1:G:105:ARG:HD3	1.91	0.52
1:1:189:ASN:HA	1:1:192:PHE:CD2	2.45	0.52
1:6:99:THR:OG1	1:6:156:MET:HB2	2.10	0.52
1:G:110:MET:HE1	1:G:116:VAL:HG23	1.92	0.52
1:G:195:ASN:OD1	1:G:196:LYS:N	2.43	0.52
1:4:157:ILE:HG23	1:5:154:TYR:HB3	1.92	0.51
1:Z:136:SER:OG	1:1:139:ILE:HG13	2.10	0.51
1:M:161:GLY:O	1:M:162:ALA:HB3	2.10	0.51
1:3:105:ARG:HH12	1:5:151:HIS:HA	1.75	0.51
1:M:162:ALA:HB1	1:M:163:PRO:HD2	1.93	0.51
1:1:182:ASN:HA	1:1:185:THR:HB	1.93	0.51
1:7:114:LYS:HA	1:7:117:ALA:HB3	1.92	0.51
1:M:196:LYS:O	1:O:195:ASN:ND2	2.43	0.51
1:R:143:SER:HA	1:R:153:ALA:HB2	1.92	0.51
1:Z:176:LEU:O	1:Z:177:PRO:C	2.47	0.51
1:1:97:ALA:HB1	1:1:131:MET:O	2.11	0.51
1:H:122:ILE:HD11	1:H:145:LEU:HD21	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:162:ALA:HB3	1:P:165:ILE:HG23	1.92	0.51
1:4:184:ILE:O	1:4:188:ILE:HG12	2.09	0.51
1:L:116:VAL:HG23	1:L:122:ILE:O	2.10	0.51
1:Y:120:ALA:O	2:Y:201:HOH:O	2.19	0.51
1:H:172:MET:HE3	1:H:176:LEU:HD21	1.92	0.51
1:3:113:GLU:HG2	1:3:114:LYS:HD3	1.93	0.51
1:Q:92:VAL:CG1	1:R:139:ILE:HG22	2.41	0.51
1:V:110:MET:HE3	1:V:112:SER:H	1.76	0.51
1:6:156:MET:O	1:6:158:ILE:O	2.29	0.50
1:6:184:ILE:CD1	1:7:188:ILE:HG23	2.42	0.50
1:N:171:ARG:O	1:N:172:MET:HB2	2.10	0.50
1:T:100:LEU:HD13	1:T:145:LEU:HD21	1.92	0.50
1:Z:154:TYR:HA	1:1:157:ILE:HD11	1.93	0.50
1:4:164:GLY:O	1:5:170:HIS:CE1	2.64	0.50
1:E:104:MET:HG2	1:E:116:VAL:HG21	1.92	0.50
1:W:105:ARG:CG	1:W:105:ARG:HH11	2.23	0.50
1:Y:176:LEU:HD21	1:Y:181:LYS:HG2	1.92	0.50
1:7:184:ILE:O	1:7:185:THR:OG1	2.22	0.50
1:C:176:LEU:HG	1:C:180:GLU:OE1	2.11	0.50
1:D:117:ALA:O	1:D:120:ALA:O	2.29	0.50
1:E:191:VAL:O	1:E:195:ASN:ND2	2.45	0.50
1:J:178:GLN:O	1:J:182:ASN:ND2	2.44	0.50
1:V:110:MET:CE	1:V:115:LYS:HG2	2.41	0.50
1:Y:186:SER:O	1:Y:189:ASN:ND2	2.44	0.50
1:Z:184:ILE:HA	1:Z:187:PHE:CE2	2.46	0.50
1:2:145:LEU:N	1:2:145:LEU:HD23	2.26	0.50
1:A:187:PHE:O	1:A:190:PHE:HB3	2.12	0.50
1:G:138:THR:HA	1:H:138:THR:HA	1.93	0.50
1:O:146:ALA:HB1	1:O:155:GLU:HG2	1.94	0.50
1:P:124:PRO:O	1:P:125:ALA:HB3	2.11	0.50
1:T:103:TRP:CZ3	1:T:156:MET:HG2	2.47	0.50
1:H:178:GLN:CD	1:H:178:GLN:H	2.15	0.50
1:Z:114:LYS:O	1:Z:117:ALA:HB3	2.11	0.50
1:3:105:ARG:NH2	1:5:154:TYR:OH	2.40	0.50
1:6:111:THR:CG2	1:6:112:SER:H	2.21	0.50
1:X:125:ALA:N	2:X:202:HOH:O	2.39	0.50
1:2:110:MET:HG3	1:2:149:PHE:CE1	2.47	0.50
1:2:136:SER:HA	1:3:139:ILE:CG1	2.42	0.50
1:B:178:GLN:O	1:B:182:ASN:OD1	2.29	0.50
1:E:106:LYS:HG2	1:E:107:ASP:H	1.76	0.50
1:G:104:MET:HA	1:G:107:ASP:HB2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:188:ILE:O	1:H:191:VAL:HG22	2.11	0.50
1:I:157:ILE:HD11	1:J:154:TYR:CA	2.40	0.50
1:Z:100:LEU:HD11	1:Z:156:MET:CE	2.42	0.50
1:B:180:GLU:HB3	2:B:201:HOH:O	2.11	0.50
1:F:100:LEU:O	1:F:104:MET:HG3	2.11	0.50
1:Q:187:PHE:CE2	1:R:184:ILE:HA	2.47	0.50
1:1:99:THR:HG21	1:1:156:MET:HA	1.93	0.50
1:3:165:ILE:HD11	1:5:105:ARG:NH2	2.27	0.50
1:C:169:ASP:OD2	1:C:171:ARG:NH2	2.40	0.50
1:I:157:ILE:HD13	1:J:153:ALA:HB3	1.93	0.50
1:U:179:GLU:HA	1:U:182:ASN:HB2	1.94	0.50
1:V:130:ILE:HD13	1:V:145:LEU:HD11	1.94	0.50
1:1:142:LEU:HD13	1:1:153:ALA:CB	2.41	0.49
1:7:126:THR:OG1	1:7:128:ASN:OD1	2.24	0.49
1:C:174:ALA:HB3	2:C:208:HOH:O	2.12	0.49
1:I:126:THR:HG22	1:I:130:ILE:HG23	1.92	0.49
1:K:185:THR:O	1:K:189:ASN:HB2	2.12	0.49
1:M:187:PHE:O	1:M:191:VAL:HG23	2.12	0.49
1:P:162:ALA:HB1	1:P:163:PRO:HD2	1.92	0.49
1:T:120:ALA:HB3	1:T:122:ILE:HG22	1.94	0.49
1:6:108:THR:O	1:6:109:GLU:HG2	2.12	0.49
1:D:173:TYR:O	1:D:181:LYS:NZ	2.45	0.49
1:H:147:ARG:NH1	2:H:203:HOH:O	2.44	0.49
1:N:176:LEU:HD22	1:N:178:GLN:NE2	2.23	0.49
1:Y:104:MET:CG	2:Y:202:HOH:O	2.59	0.49
1:Z:146:ALA:HB2	2:Z:201:HOH:O	2.11	0.49
1:K:184:ILE:HG13	1:K:185:THR:H	1.76	0.49
1:4:142:LEU:HA	1:4:145:LEU:HG	1.93	0.49
1:7:126:THR:CB	1:7:128:ASN:OD1	2.61	0.49
1:A:112:SER:O	2:A:201:HOH:O	2.20	0.49
1:Q:109:GLU:HG3	1:Q:110:MET:N	2.27	0.49
1:2:157:ILE:CD1	1:3:154:TYR:HA	2.43	0.49
1:3:92:VAL:N	2:3:202:HOH:O	2.46	0.49
1:6:168:TYR:CE2	1:6:170:HIS:HD2	2.30	0.49
1:F:180:GLU:HA	1:F:183:LYS:HE2	1.93	0.49
1:P:149:PHE:HA	2:P:205:HOH:O	2.11	0.49
1:Y:110:MET:HG2	1:Y:111:THR:HG23	1.95	0.49
1:3:117:ALA:O	1:3:121:GLY:N	2.45	0.49
1:E:181:LYS:NZ	2:E:203:HOH:O	2.45	0.49
1:E:166:ILE:HG12	1:F:173:TYR:CZ	2.48	0.49
1:O:95:GLN:HE22	1:O:159:PRO:HA	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:151:HIS:CE1	1:5:106:LYS:HA	2.47	0.49
1:4:168:TYR:CE2	1:5:165:ILE:HG13	2.46	0.49
1:C:120:ALA:HB2	1:C:145:LEU:HD23	1.95	0.49
1:E:136:SER:HB3	1:F:138:THR:CG2	2.39	0.49
1:K:122:ILE:HG22	1:K:124:PRO:HD2	1.95	0.49
1:K:184:ILE:CG2	1:L:166:ILE:HG23	2.43	0.49
1:H:190:PHE:O	1:H:193:GLU:HG3	2.13	0.49
1:2:136:SER:C	1:3:138:THR:HG1	2.15	0.49
1:7:123:GLY:O	1:7:125:ALA:N	2.41	0.49
1:F:110:MET:HB3	1:F:116:VAL:HG22	1.95	0.49
1:M:130:ILE:O	1:M:131:MET:C	2.51	0.49
1:U:101:ASN:OD1	1:U:105:ARG:NH2	2.46	0.49
1:Z:139:ILE:HG12	1:1:137:THR:O	2.13	0.49
1:B:122:ILE:HG22	1:B:123:GLY:H	1.77	0.49
1:E:117:ALA:HB2	1:E:127:VAL:HG21	1.95	0.49
1:J:130:ILE:HG12	1:J:137:THR:OG1	2.13	0.49
1:N:180:GLU:O	1:W:183:LYS:NZ	2.42	0.49
1:Q:168:TYR:CE2	1:Q:170:HIS:CD2	3.01	0.49
1:R:177:PRO:HA	1:T:105:ARG:HH12	1.76	0.49
1:V:173:TYR:O	1:V:181:LYS:NZ	2.45	0.49
1:3:161:GLY:HA2	1:5:132:LYS:HG3	1.95	0.48
1:6:168:TYR:CZ	1:6:170:HIS:HD2	2.30	0.48
1:A:179:GLU:O	1:A:183:LYS:HG2	2.13	0.48
1:C:110:MET:SD	1:C:115:LYS:NZ	2.77	0.48
1:F:165:ILE:HD12	1:F:165:ILE:N	2.28	0.48
1:K:158:ILE:O	1:K:158:ILE:HG22	2.12	0.48
1:F:183:LYS:HG2	1:5:183:LYS:HG2	1.95	0.48
1:6:157:ILE:HG12	1:7:154:TYR:HB3	1.94	0.48
1:I:126:THR:O	1:I:130:ILE:HG23	2.13	0.48
1:K:159:PRO:O	1:K:165:ILE:HD11	2.13	0.48
1:O:125:ALA:O	1:O:128:ASN:ND2	2.46	0.48
1:4:110:MET:HE1	1:4:115:LYS:HB3	1.96	0.48
1:M:187:PHE:HE2	1:N:183:LYS:O	1.96	0.48
1:X:107:ASP:CG	1:X:110:MET:H	2.16	0.48
1:N:190:PHE:O	1:N:191:VAL:C	2.52	0.48
1:Q:92:VAL:HG13	1:Q:157:ILE:CG2	2.44	0.48
1:7:172:MET:O	1:7:174:ALA:N	2.47	0.48
1:J:146:ALA:HB1	1:J:151:HIS:O	2.12	0.48
1:W:106:LYS:NZ	2:W:202:HOH:O	2.34	0.48
1:Y:112:SER:N	2:Y:202:HOH:O	2.22	0.48
1:3:154:TYR:CE2	1:3:155:GLU:HG2	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:100:LEU:HB2	2:5:209:HOH:O	2.13	0.48
1:5:155:GLU:O	1:5:155:GLU:HG3	2.13	0.48
1:6:151:HIS:CD2	1:6:152:GLU:N	2.82	0.48
1:F:94:LYS:NZ	2:F:205:HOH:O	2.45	0.48
1:I:187:PHE:O	1:I:190:PHE:HB3	2.14	0.48
1:J:104:MET:O	1:J:110:MET:HA	2.13	0.48
1:N:173:TYR:CE2	1:N:181:LYS:HD2	2.49	0.48
1:N:173:TYR:CE2	1:N:183:LYS:CG	2.93	0.48
1:Q:176:LEU:HG	1:Q:180:GLU:OE2	2.13	0.48
1:V:99:THR:HG22	1:V:103:TRP:CE2	2.48	0.48
1:3:165:ILE:HD11	1:5:105:ARG:HH22	1.79	0.48
1:P:190:PHE:C	1:P:191:VAL:HG22	2.33	0.48
1:E:163:PRO:HB3	1:G:98:ALA:HB2	1.96	0.48
1:K:116:VAL:O	1:K:116:VAL:HG23	2.14	0.48
1:M:187:PHE:HA	1:W:190:PHE:CE1	2.48	0.48
1:O:104:MET:O	1:O:111:THR:HG23	2.13	0.48
1:O:99:THR:HG21	1:O:156:MET:HA	1.96	0.48
1:P:96:ALA:N	2:P:201:HOH:O	2.46	0.48
1:U:162:ALA:HB2	1:W:105:ARG:CZ	2.44	0.48
1:X:125:ALA:O	1:X:128:ASN:HB3	2.14	0.48
1:1:160:VAL:HG11	1:7:97:ALA:HB3	1.95	0.47
1:Z:164:GLY:HA2	1:1:173:TYR:CD1	2.48	0.47
1:4:157:ILE:HG21	1:5:153:ALA:HB3	1.96	0.47
1:5:170:HIS:O	1:5:170:HIS:CG	2.66	0.47
1:1:151:HIS:NE2	1:7:106:LYS:HG2	2.29	0.47
1:C:111:THR:OG1	1:C:112:SER:N	2.47	0.47
1:C:125:ALA:O	1:C:129:ARG:N	2.37	0.47
1:E:167:ASP:OD1	1:E:167:ASP:N	2.47	0.47
1:N:124:PRO:HA	1:N:127:VAL:HG12	1.96	0.47
1:Q:188:ILE:HG22	1:Q:192:PHE:CZ	2.49	0.47
1:T:174:ALA:HA	1:T:181:LYS:HZ1	1.77	0.47
1:E:172:MET:SD	1:F:192:PHE:CE2	3.07	0.47
1:V:99:THR:HG21	1:V:156:MET:HA	1.96	0.47
1:Z:96:ALA:C	1:Z:100:LEU:HD13	2.35	0.47
1:Z:115:LYS:O	1:Z:118:VAL:HG12	2.15	0.47
1:G:113:GLU:O	1:G:114:LYS:HG3	2.15	0.47
1:N:157:ILE:O	1:N:159:PRO:HD3	2.14	0.47
1:O:159:PRO:HB2	1:O:162:ALA:HA	1.95	0.47
1:U:128:ASN:OD1	1:U:132:LYS:HD3	2.14	0.47
1:G:173:TYR:O	1:G:181:LYS:HE2	2.15	0.47
1:W:107:ASP:OD1	1:W:108:THR:N	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:103:TRP:CE2	1:Z:151:HIS:CD2	3.02	0.47
1:1:142:LEU:HD12	1:1:143:SER:N	2.28	0.47
1:3:137:THR:CG2	1:3:141:VAL:HG23	2.45	0.47
1:K:184:ILE:HG13	1:K:185:THR:N	2.29	0.47
1:N:171:ARG:CG	1:N:172:MET:H	2.27	0.47
1:P:110:MET:O	1:P:111:THR:HG22	2.13	0.47
1:T:126:THR:HA	1:T:129:ARG:HE	1.79	0.47
1:V:110:MET:HG3	1:V:116:VAL:HG13	1.96	0.47
1:6:184:ILE:HG12	1:7:188:ILE:HG13	1.97	0.47
1:G:116:VAL:O	1:G:120:ALA:N	2.42	0.47
1:O:193:GLU:N	1:O:193:GLU:OE1	2.47	0.47
1:5:111:THR:OG1	1:5:116:VAL:HG13	2.14	0.47
1:5:114:LYS:CG	1:5:128:ASN:OD1	2.63	0.47
1:C:104:MET:HE3	1:C:131:MET:SD	2.55	0.47
1:P:111:THR:O	1:P:112:SER:CB	2.62	0.47
1:Q:162:ALA:HB1	1:Q:163:PRO:HD2	1.96	0.47
1:Y:194:GLN:HG2	1:Y:195:ASN:ND2	2.30	0.47
1:3:92:VAL:HB	1:3:93:GLU:OE1	2.14	0.47
1:5:172:MET:HG2	1:5:173:TYR:CD1	2.50	0.47
1:K:184:ILE:HG22	1:L:166:ILE:HG23	1.95	0.47
1:M:193:GLU:O	1:M:196:LYS:HB3	2.15	0.47
1:X:143:SER:CB	1:Y:92:VAL:HG21	2.45	0.47
1:5:170:HIS:O	1:5:173:TYR:CD2	2.68	0.47
1:6:157:ILE:HD11	1:7:153:ALA:HB1	1.97	0.47
1:D:191:VAL:O	1:D:191:VAL:CG1	2.63	0.47
1:I:126:THR:HA	1:I:129:ARG:HB2	1.96	0.47
1:L:99:THR:HG21	1:L:156:MET:HA	1.97	0.47
1:P:119:ALA:HB2	1:P:148:ALA:HB2	1.97	0.47
1:T:102:ALA:O	1:T:105:ARG:HG2	2.15	0.47
1:Y:122:ILE:HD11	1:Y:127:VAL:HG22	1.97	0.47
1:P:177:PRO:HB2	1:Y:179:GLU:OE1	2.15	0.47
1:4:182:ASN:O	1:4:186:SER:OG	2.31	0.47
1:5:113:GLU:HB3	1:5:128:ASN:CG	2.34	0.47
1:I:110:MET:HE2	1:I:114:LYS:HG3	1.97	0.47
1:K:157:ILE:HG21	1:L:154:TYR:CD1	2.50	0.47
1:Q:180:GLU:O	1:Q:183:LYS:HB2	2.15	0.47
1:W:117:ALA:HA	1:W:122:ILE:HG22	1.97	0.47
1:X:146:ALA:O	1:X:151:HIS:N	2.44	0.47
1:Y:187:PHE:O	1:Y:190:PHE:HD1	1.98	0.47
1:1:194:GLN:NE2	2:1:202:HOH:O	2.47	0.46
1:5:114:LYS:O	1:5:118:VAL:N	2.43	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:168:TYR:CZ	1:C:170:HIS:CE1	3.03	0.46
1:D:112:SER:HB3	1:D:115:LYS:HG3	1.96	0.46
1:D:143:SER:HA	1:D:153:ALA:HB2	1.96	0.46
1:R:170:HIS:O	1:R:174:ALA:N	2.44	0.46
1:U:192:PHE:HA	1:U:193:GLU:CG	2.44	0.46
1:6:98:ALA:N	1:6:156:MET:CE	2.79	0.46
1:7:183:LYS:NZ	1:7:184:ILE:HG22	2.30	0.46
1:F:154:TYR:O	1:F:158:ILE:HG13	2.14	0.46
1:G:154:TYR:O	1:G:158:ILE:HG23	2.15	0.46
1:G:194:GLN:NE2	1:7:179:GLU:O	2.48	0.46
1:H:182:ASN:HA	1:H:185:THR:OG1	2.15	0.46
1:U:92:VAL:N	2:U:208:HOH:O	2.47	0.46
1:6:96:ALA:HA	1:6:156:MET:HB3	1.96	0.46
1:A:100:LEU:HD23	1:A:100:LEU:C	2.35	0.46
1:M:139:ILE:HA	1:M:142:LEU:HD12	1.97	0.46
1:O:190:PHE:CG	1:O:191:VAL:N	2.84	0.46
1:P:187:PHE:CE1	1:P:190:PHE:CD2	3.03	0.46
1:R:185:THR:CB	2:R:201:HOH:O	2.61	0.46
1:U:113:GLU:OE2	1:U:128:ASN:HB2	2.15	0.46
1:2:125:ALA:O	1:2:129:ARG:N	2.47	0.46
1:4:103:TRP:HB3	1:4:149:PHE:CD2	2.51	0.46
1:4:155:GLU:OE1	1:4:170:HIS:CG	2.69	0.46
1:5:138:THR:HG23	1:5:141:VAL:H	1.80	0.46
1:E:173:TYR:CZ	1:F:166:ILE:HG12	2.50	0.46
1:K:155:GLU:O	1:K:158:ILE:HD12	2.14	0.46
1:N:129:ARG:NH2	1:N:134:GLU:OE1	2.49	0.46
1:Q:92:VAL:CG1	1:R:139:ILE:CG2	2.94	0.46
1:1:149:PHE:HD1	1:7:106:LYS:HZ2	1.62	0.46
1:K:171:ARG:O	1:K:174:ALA:HB3	2.16	0.46
1:P:179:GLU:O	1:Y:183:LYS:NZ	2.48	0.46
1:R:178:GLN:O	1:R:182:ASN:OD1	2.34	0.46
1:5:170:HIS:O	1:5:171:ARG:HB2	2.16	0.46
1:A:117:ALA:O	1:A:121:GLY:N	2.48	0.46
1:C:112:SER:O	1:C:115:LYS:HB3	2.15	0.46
1:K:154:TYR:CE1	1:L:159:PRO:HD3	2.51	0.46
1:1:188:ILE:HA	1:1:191:VAL:HG22	1.97	0.46
1:2:122:ILE:HD12	1:2:122:ILE:N	2.30	0.46
1:5:92:VAL:HB	1:5:93:GLU:OE1	2.16	0.46
1:7:126:THR:HB	1:7:128:ASN:OD1	2.15	0.46
1:G:114:LYS:C	1:G:116:VAL:N	2.69	0.46
1:I:191:VAL:HG23	1:I:196:LYS:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:154:TYR:CZ	1:L:159:PRO:HD3	2.50	0.46
1:N:112:SER:O	1:N:116:VAL:HG13	2.16	0.46
1:N:158:ILE:HG23	1:N:158:ILE:O	2.16	0.46
1:X:191:VAL:O	1:X:195:ASN:OD1	2.33	0.46
1:2:104:MET:HG3	1:2:105:ARG:HG2	1.98	0.46
1:3:122:ILE:HG22	1:3:123:GLY:N	2.31	0.46
1:6:98:ALA:N	1:6:156:MET:HE3	2.30	0.46
1:7:103:TRP:CZ3	1:7:156:MET:SD	3.09	0.46
1:C:161:GLY:N	2:C:203:HOH:O	2.38	0.46
1:D:125:ALA:O	1:D:129:ARG:HG3	2.16	0.46
1:N:115:LYS:HA	1:N:118:VAL:HG22	1.96	0.46
1:N:127:VAL:HA	1:N:130:ILE:HD13	1.97	0.46
1:O:185:THR:O	1:O:188:ILE:HG12	2.15	0.46
1:6:139:ILE:HD13	2:7:201:HOH:O	2.15	0.46
1:H:117:ALA:HB1	1:H:122:ILE:O	2.16	0.46
1:T:117:ALA:HA	1:T:122:ILE:HG23	1.98	0.46
1:T:136:SER:HB3	1:U:138:THR:HB	1.98	0.46
1:2:168:TYR:CZ	1:3:166:ILE:HD11	2.51	0.46
1:6:152:GLU:CG	1:6:153:ALA:H	2.29	0.46
1:C:114:LYS:O	1:C:118:VAL:HG23	2.16	0.46
1:E:138:THR:HG23	1:F:136:SER:OG	2.16	0.46
1:G:193:GLU:HA	1:G:195:ASN:OD1	2.15	0.46
1:K:120:ALA:HB2	1:K:127:VAL:HG12	1.97	0.46
1:K:97:ALA:HB1	1:K:131:MET:SD	2.56	0.46
1:3:167:ASP:OD2	1:5:113:GLU:OE1	2.34	0.45
1:6:94:LYS:N	1:6:133:ALA:CB	2.78	0.45
1:L:116:VAL:HG21	1:L:127:VAL:HG21	1.98	0.45
1:Y:173:TYR:O	1:Y:181:LYS:HE2	2.16	0.45
1:G:149:PHE:HB2	1:G:151:HIS:HD2	1.81	0.45
1:M:157:ILE:CD1	1:N:154:TYR:HB3	2.46	0.45
1:1:103:TRP:CD1	1:7:102:ALA:HB1	2.51	0.45
1:7:170:HIS:CD2	1:7:173:TYR:CD2	3.04	0.45
1:G:129:ARG:HB2	1:G:135:VAL:HG22	1.99	0.45
1:G:93:GLU:HG2	1:G:136:SER:HA	1.99	0.45
1:P:119:ALA:CB	1:P:148:ALA:HB2	2.47	0.45
1:4:187:PHE:CE2	1:5:184:ILE:HA	2.50	0.45
1:5:146:ALA:HB1	1:5:151:HIS:O	2.16	0.45
1:6:163:PRO:HB2	1:7:178:GLN:OE1	2.16	0.45
1:E:104:MET:HA	1:E:110:MET:O	2.16	0.45
1:P:157:ILE:HA	2:P:201:HOH:O	2.15	0.45
1:Q:92:VAL:N	2:Q:202:HOH:O	2.48	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:171:ARG:NH1	1:T:132:LYS:O	2.50	0.45
1:F:162:ALA:HB1	1:F:165:ILE:HB	1.99	0.45
1:J:129:ARG:HG2	1:J:134:GLU:HB2	1.98	0.45
1:Z:129:ARG:NH2	1:Z:134:GLU:CD	2.70	0.45
1:1:112:SER:CB	1:1:115:LYS:HE2	2.46	0.45
1:2:110:MET:CE	1:2:148:ALA:HB1	2.47	0.45
1:H:190:PHE:C	1:H:190:PHE:CD1	2.90	0.45
1:R:107:ASP:OD1	1:R:108:THR:N	2.49	0.45
1:Y:108:THR:C	1:Y:110:MET:H	2.19	0.45
1:3:178:GLN:HA	1:3:181:LYS:CE	2.45	0.45
1:4:92:VAL:O	1:5:139:ILE:HD13	2.17	0.45
1:6:132:LYS:NZ	1:6:132:LYS:H	2.15	0.45
1:G:173:TYR:CE2	1:H:166:ILE:HG12	2.52	0.45
1:I:103:TRP:HH2	1:I:156:MET:SD	2.39	0.45
1:Z:103:TRP:CZ2	1:Z:151:HIS:CD2	3.05	0.45
1:3:111:THR:HG21	1:5:168:TYR:HA	1.99	0.45
1:3:138:THR:CG2	1:3:141:VAL:HG22	2.45	0.45
1:4:99:THR:HG21	1:4:156:MET:HB3	1.98	0.45
1:D:101:ASN:HD21	1:F:160:VAL:HA	1.81	0.45
1:L:116:VAL:HG11	1:L:127:VAL:CG2	2.47	0.45
1:W:177:PRO:O	1:W:181:LYS:N	2.49	0.45
1:Y:178:GLN:O	1:Y:181:LYS:HB2	2.16	0.45
1:6:157:ILE:HG23	1:7:154:TYR:HB3	1.97	0.45
1:6:161:GLY:C	1:6:163:PRO:HD3	2.37	0.45
1:G:176:LEU:O	1:G:181:LYS:HE3	2.17	0.45
1:H:177:PRO:O	1:H:181:LYS:HG3	2.17	0.45
1:M:128:ASN:OD1	1:M:128:ASN:C	2.55	0.45
1:O:195:ASN:HD21	1:P:175:ALA:HB2	1.81	0.45
1:P:183:LYS:O	1:P:187:PHE:HB3	2.16	0.45
1:R:105:ARG:HA	1:R:111:THR:HG22	1.98	0.45
1:V:116:VAL:HG23	1:V:117:ALA:N	2.32	0.45
1:W:134:GLU:HB2	2:W:201:HOH:O	2.16	0.45
1:2:120:ALA:HB1	1:2:145:LEU:HD22	1.98	0.45
1:3:182:ASN:HA	1:3:185:THR:HB	1.99	0.45
1:D:145:LEU:O	1:D:148:ALA:HB3	2.17	0.45
1:F:117:ALA:HB1	1:F:122:ILE:O	2.17	0.45
1:G:122:ILE:HD11	1:G:127:VAL:HG22	1.99	0.45
1:I:129:ARG:HB3	1:I:134:GLU:CG	2.46	0.45
1:G:92:VAL:N	2:G:204:HOH:O	2.49	0.44
1:L:168:TYR:CD1	1:L:168:TYR:O	2.70	0.44
1:O:169:ASP:HB3	1:O:172:MET:HA	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:164:GLY:O	1:Y:168:TYR:HE1	2.01	0.44
1:6:132:LYS:O	1:6:133:ALA:CB	2.64	0.44
1:A:102:ALA:HA	1:A:105:ARG:HD3	1.99	0.44
1:C:104:MET:CE	1:C:131:MET:SD	3.05	0.44
1:E:185:THR:HA	1:E:188:ILE:HD12	1.99	0.44
1:I:103:TRP:CH2	1:I:156:MET:SD	3.10	0.44
1:X:143:SER:HA	1:X:153:ALA:HB2	1.99	0.44
1:Y:187:PHE:O	1:Y:190:PHE:CD1	2.70	0.44
1:Z:151:HIS:NE2	1:Z:170:HIS:O	2.49	0.44
1:2:168:TYR:CZ	1:2:170:HIS:CE1	3.06	0.44
1:4:141:VAL:HG12	1:4:145:LEU:HD23	1.98	0.44
1:B:112:SER:HB2	1:B:115:LYS:HB2	1.98	0.44
1:E:138:THR:HG22	1:E:141:VAL:H	1.82	0.44
1:J:102:ALA:HA	1:J:105:ARG:NH2	2.32	0.44
1:M:96:ALA:HB2	1:M:157:ILE:HG22	1.98	0.44
1:P:103:TRP:HB3	1:P:149:PHE:CD1	2.52	0.44
1:Q:146:ALA:HB2	1:Q:156:MET:HE2	2.00	0.44
1:Q:92:VAL:HG13	1:Q:157:ILE:HG23	1.98	0.44
1:U:191:VAL:C	1:U:193:GLU:HA	2.37	0.44
1:W:192:PHE:O	1:W:196:LYS:N	2.46	0.44
1:Z:157:ILE:HG13	1:1:154:TYR:CZ	2.52	0.44
1:2:104:MET:SD	1:2:131:MET:HG2	2.58	0.44
1:2:151:HIS:CE1	1:2:171:ARG:HB2	2.53	0.44
1:4:113:GLU:O	1:4:114:LYS:HD2	2.18	0.44
1:K:104:MET:HG2	1:K:149:PHE:CZ	2.52	0.44
1:G:157:ILE:HD12	1:H:157:ILE:HD11	2.00	0.44
1:O:178:GLN:O	1:O:179:GLU:C	2.55	0.44
1:V:110:MET:HG2	1:V:116:VAL:CG1	2.46	0.44
1:V:143:SER:HA	1:V:153:ALA:HB2	2.00	0.44
1:Z:113:GLU:O	1:Z:116:VAL:HG12	2.18	0.44
1:4:168:TYR:OH	1:4:170:HIS:NE2	2.45	0.44
1:4:181:LYS:O	1:4:185:THR:OG1	2.28	0.44
1:B:173:TYR:CZ	1:B:181:LYS:CD	3.00	0.44
1:E:93:GLU:HG3	1:F:139:ILE:HD11	1.99	0.44
1:I:157:ILE:HD11	1:J:153:ALA:C	2.37	0.44
1:Q:162:ALA:HB3	1:Q:165:ILE:HD12	1.98	0.44
1:4:154:TYR:CD1	1:5:159:PRO:HD2	2.53	0.44
1:7:184:ILE:HB	2:7:206:HOH:O	2.17	0.44
1:C:189:ASN:ND2	1:C:193:GLU:OE2	2.51	0.44
1:3:93:GLU:N	1:3:93:GLU:OE1	2.47	0.44
1:A:161:GLY:O	1:A:162:ALA:C	2.55	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:142:LEU:HD11	1:P:156:MET:HE2	2.00	0.44
1:Z:176:LEU:CG	1:Z:177:PRO:HD2	2.39	0.44
1:A:166:ILE:HG12	1:B:173:TYR:CE1	2.53	0.44
1:X:120:ALA:HB3	1:X:122:ILE:HG12	1.99	0.44
1:6:173:TYR:HB2	1:6:176:LEU:HD13	2.00	0.43
1:G:111:THR:OG1	1:G:112:SER:N	2.50	0.43
1:I:122:ILE:HG21	1:I:145:LEU:HD11	1.99	0.43
1:P:117:ALA:HB1	1:P:122:ILE:O	2.18	0.43
1:Q:143:SER:HA	1:Q:153:ALA:HB2	1.99	0.43
1:W:105:ARG:NH1	1:W:105:ARG:CG	2.80	0.43
1:3:113:GLU:HG2	1:3:114:LYS:CD	2.48	0.43
1:4:168:TYR:HD2	1:4:172:MET:HE1	1.83	0.43
1:4:168:TYR:CZ	1:5:165:ILE:HG13	2.53	0.43
1:B:169:ASP:C	1:B:169:ASP:OD1	2.55	0.43
1:C:104:MET:HE2	1:C:104:MET:HB2	1.64	0.43
1:N:143:SER:CA	1:N:153:ALA:HB2	2.43	0.43
1:N:178:GLN:OE1	1:N:181:LYS:CD	2.66	0.43
1:P:126:THR:HG22	1:P:128:ASN:N	2.33	0.43
1:Q:173:TYR:CZ	1:R:166:ILE:HG12	2.53	0.43
1:V:110:MET:SD	1:V:115:LYS:CG	3.06	0.43
1:6:162:ALA:N	1:6:163:PRO:CD	2.80	0.43
1:7:170:HIS:CD2	1:7:171:ARG:N	2.87	0.43
1:A:99:THR:HA	1:A:102:ALA:HB3	2.00	0.43
1:E:101:ASN:OD1	1:E:131:MET:SD	2.76	0.43
1:F:177:PRO:HA	1:G:105:ARG:CZ	2.49	0.43
1:G:162:ALA:N	2:G:203:HOH:O	2.47	0.43
1:O:173:TYR:CZ	1:P:191:VAL:HG23	2.54	0.43
1:V:97:ALA:CB	1:V:133:ALA:HB2	2.47	0.43
1:2:110:MET:HE1	1:2:148:ALA:HB1	2.00	0.43
1:M:170:HIS:CD2	1:M:170:HIS:O	2.71	0.43
1:O:152:GLU:O	1:O:155:GLU:HG3	2.19	0.43
1:V:116:VAL:HG23	1:V:127:VAL:HG21	2.01	0.43
1:X:125:ALA:O	1:X:129:ARG:HG2	2.19	0.43
1:C:143:SER:O	1:C:147:ARG:HG3	2.17	0.43
1:K:108:THR:OG1	1:K:109:GLU:N	2.50	0.43
1:K:111:THR:OG1	1:K:112:SER:N	2.48	0.43
1:T:173:TYR:C	1:T:173:TYR:CD1	2.92	0.43
1:F:110:MET:SD	1:F:116:VAL:HA	2.58	0.43
1:H:180:GLU:HA	1:H:180:GLU:OE1	2.19	0.43
1:K:114:LYS:HA	1:K:127:VAL:HG23	2.00	0.43
1:V:98:ALA:HB2	1:X:163:PRO:HB3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:92:VAL:CG2	1:G:157:ILE:HG23	2.49	0.43
1:H:130:ILE:HG12	1:H:137:THR:OG1	2.19	0.43
1:G:187:PHE:CD2	1:H:187:PHE:CD2	3.07	0.43
1:I:96:ALA:HB2	1:I:157:ILE:HG22	2.01	0.43
1:Z:128:ASN:OD1	1:Z:131:MET:CE	2.67	0.43
1:Z:100:LEU:CD1	1:Z:156:MET:HE3	2.48	0.43
1:3:95:GLN:N	2:3:202:HOH:O	2.52	0.43
1:H:106:LYS:O	1:H:107:ASP:CB	2.66	0.43
1:I:120:ALA:HB3	1:I:122:ILE:HG13	2.01	0.43
1:J:172:MET:HG3	1:J:175:ALA:CB	2.47	0.43
1:K:183:LYS:CG	1:K:184:ILE:N	2.81	0.43
1:R:113:GLU:HG3	1:R:114:LYS:N	2.33	0.43
1:3:171:ARG:C	1:3:173:TYR:N	2.72	0.43
1:6:99:THR:HG22	1:6:103:TRP:CE2	2.54	0.43
1:6:162:ALA:N	1:6:163:PRO:HD3	2.34	0.43
1:B:125:ALA:N	2:B:205:HOH:O	2.47	0.43
1:M:127:VAL:HA	1:M:130:ILE:HG22	2.00	0.43
1:M:182:ASN:O	1:M:183:LYS:C	2.56	0.43
1:V:134:GLU:CG	1:Y:171:ARG:NH2	2.82	0.43
1:V:122:ILE:HD12	1:V:141:VAL:HG22	2.00	0.43
1:4:136:SER:HG	1:5:140:GLY:H	1.63	0.43
1:C:103:TRP:HB3	1:C:149:PHE:CZ	2.54	0.43
1:E:176:LEU:HD21	1:F:192:PHE:HD1	1.82	0.43
1:N:128:ASN:ND2	2:N:205:HOH:O	2.45	0.43
1:W:189:ASN:O	1:W:192:PHE:HB2	2.19	0.43
1:X:164:GLY:H	1:Y:170:HIS:CE1	2.37	0.43
1:1:189:ASN:HA	1:1:192:PHE:CE2	2.54	0.42
1:2:158:ILE:HD13	1:3:154:TYR:CG	2.54	0.42
1:F:130:ILE:HD13	1:F:145:LEU:HD11	2.00	0.42
1:O:152:GLU:HG3	1:P:163:PRO:HG3	2.01	0.42
1:Y:104:MET:HG3	2:Y:202:HOH:O	2.19	0.42
1:Z:122:ILE:HG22	1:Z:123:GLY:H	1.83	0.42
1:2:184:ILE:HG12	1:3:187:PHE:HE2	1.84	0.42
1:E:173:TYR:CZ	1:E:181:LYS:HD2	2.54	0.42
1:M:97:ALA:CA	1:M:131:MET:HB3	2.48	0.42
1:M:192:PHE:CZ	1:W:186:SER:HB2	2.54	0.42
1:N:107:ASP:O	1:N:110:MET:HG3	2.19	0.42
1:N:147:ARG:NH2	1:N:152:GLU:OE1	2.51	0.42
1:N:178:GLN:O	1:N:181:LYS:HD3	2.19	0.42
1:R:171:ARG:NE	2:R:204:HOH:O	2.51	0.42
1:R:97:ALA:O	1:R:101:ASN:ND2	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:183:LYS:NZ	2:V:204:HOH:O	2.53	0.42
1:6:157:ILE:HG23	1:7:154:TYR:HB2	2.00	0.42
1:D:101:ASN:ND2	1:F:160:VAL:HA	2.33	0.42
1:G:111:THR:HG23	1:G:116:VAL:CG1	2.49	0.42
1:I:187:PHE:CE2	1:I:190:PHE:CG	3.08	0.42
1:M:128:ASN:OD1	1:M:129:ARG:HG3	2.18	0.42
1:V:132:LYS:O	1:V:133:ALA:HB3	2.19	0.42
1:2:97:ALA:O	1:2:101:ASN:ND2	2.52	0.42
1:3:158:ILE:O	1:3:158:ILE:HG13	2.19	0.42
1:B:108:THR:C	1:B:110:MET:H	2.22	0.42
1:D:111:THR:OG1	1:F:167:ASP:OD2	2.34	0.42
1:H:186:SER:HA	1:H:189:ASN:HB2	2.01	0.42
1:Q:153:ALA:HA	1:Q:156:MET:HE2	2.01	0.42
1:2:173:TYR:OH	1:3:166:ILE:HG23	2.19	0.42
1:6:136:SER:OG	1:7:140:GLY:N	2.51	0.42
1:G:95:GLN:HG3	1:G:156:MET:O	2.19	0.42
1:N:152:GLU:HB3	1:N:155:GLU:HG3	2.02	0.42
1:M:192:PHE:HZ	1:W:186:SER:HB2	1.83	0.42
1:Z:126:THR:N	1:Z:127:VAL:HG22	2.35	0.42
1:Z:93:GLU:N	1:Z:93:GLU:OE1	2.39	0.42
1:2:139:ILE:HD11	1:3:142:LEU:HD22	2.02	0.42
1:3:160:VAL:HG13	1:5:131:MET:O	2.19	0.42
1:6:168:TYR:OH	1:7:166:ILE:HD11	2.20	0.42
1:A:142:LEU:HA	2:A:208:HOH:O	2.19	0.42
1:K:105:ARG:HA	1:K:107:ASP:HB2	2.01	0.42
1:K:145:LEU:C	1:K:145:LEU:HD23	2.39	0.42
1:M:97:ALA:CB	1:M:131:MET:HB3	2.50	0.42
1:W:122:ILE:HD11	1:W:126:THR:HB	2.02	0.42
1:Z:100:LEU:HD11	1:Z:156:MET:HE3	2.01	0.42
1:A:195:ASN:ND2	1:B:180:GLU:OE2	2.50	0.42
1:I:158:ILE:HG22	1:J:154:TYR:CG	2.54	0.42
1:N:94:LYS:N	1:N:94:LYS:HD2	2.34	0.42
1:T:173:TYR:HB2	1:U:192:PHE:HZ	1.84	0.42
1:6:171:ARG:O	1:6:172:MET:C	2.57	0.42
1:7:112:SER:O	1:7:115:LYS:HG3	2.19	0.42
1:F:130:ILE:HG12	1:F:137:THR:HG21	2.00	0.42
1:I:187:PHE:CE2	1:I:190:PHE:CD1	3.08	0.42
1:I:157:ILE:CD1	1:J:153:ALA:HB3	2.50	0.42
1:I:154:TYR:HB3	1:J:158:ILE:HA	2.02	0.42
1:L:188:ILE:O	1:L:191:VAL:HG22	2.19	0.42
1:O:137:THR:HG22	1:O:138:THR:N	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:187:PHE:O	1:X:191:VAL:HG23	2.19	0.42
1:Z:97:ALA:HB2	1:Z:133:ALA:CB	2.50	0.42
1:Z:171:ARG:HG3	1:1:164:GLY:CA	2.37	0.42
1:1:160:VAL:HG11	1:7:97:ALA:CB	2.49	0.42
1:2:96:ALA:CB	1:2:100:LEU:HD23	2.44	0.42
1:7:162:ALA:HB1	1:7:163:PRO:CA	2.42	0.42
1:H:176:LEU:O	1:H:181:LYS:NZ	2.49	0.42
1:O:103:TRP:HB3	1:O:149:PHE:CE2	2.55	0.42
1:2:104:MET:CG	1:2:105:ARG:N	2.83	0.42
1:3:100:LEU:HD13	1:3:145:LEU:HD23	2.02	0.42
1:5:115:LYS:HA	1:5:118:VAL:HG22	2.01	0.42
1:G:122:ILE:CD1	1:G:145:LEU:HD21	2.49	0.42
1:H:110:MET:HB3	1:H:115:LYS:HG3	2.00	0.42
1:K:162:ALA:HB1	1:K:163:PRO:HD2	2.02	0.42
1:M:97:ALA:HB2	1:M:131:MET:C	2.41	0.42
1:P:116:VAL:HG12	1:P:145:LEU:HD11	2.01	0.42
1:1:184:ILE:O	1:1:188:ILE:HG12	2.20	0.41
1:3:157:ILE:HG22	1:3:157:ILE:O	2.20	0.41
1:6:103:TRP:CZ2	1:6:151:HIS:ND1	2.86	0.41
1:F:92:VAL:N	2:F:206:HOH:O	2.52	0.41
1:O:174:ALA:O	1:O:181:LYS:CE	2.67	0.41
1:2:122:ILE:HD11	1:2:145:LEU:HD21	2.03	0.41
1:B:112:SER:N	2:B:206:HOH:O	2.54	0.41
1:G:111:THR:CG2	1:G:116:VAL:HG12	2.50	0.41
1:G:136:SER:HB2	1:H:138:THR:CG2	2.50	0.41
1:G:148:ALA:N	2:G:207:HOH:O	2.53	0.41
1:R:194:GLN:NE2	1:Z:183:LYS:HD3	2.35	0.41
1:1:105:ARG:NH1	2:1:204:HOH:O	2.53	0.41
1:4:142:LEU:HD23	1:4:153:ALA:HB1	2.01	0.41
1:C:164:GLY:HA3	1:D:170:HIS:HB3	2.02	0.41
1:I:157:ILE:HG12	1:J:157:ILE:HD11	2.02	0.41
1:I:168:TYR:CE1	1:J:166:ILE:HD12	2.55	0.41
1:K:174:ALA:HB2	1:L:163:PRO:CB	2.50	0.41
1:M:103:TRP:CZ3	1:M:156:MET:HG2	2.55	0.41
1:N:182:ASN:HB3	1:N:186:SER:CA	2.51	0.41
1:Z:169:ASP:OD1	1:Z:170:HIS:N	2.53	0.41
1:Z:94:LYS:O	1:Z:97:ALA:N	2.52	0.41
1:J:162:ALA:O	1:J:165:ILE:HG12	2.19	0.41
1:K:159:PRO:O	1:K:165:ILE:CD1	2.69	0.41
1:P:97:ALA:HB2	1:P:131:MET:O	2.20	0.41
1:U:155:GLU:HA	1:U:158:ILE:CD1	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4:173:TYR:CD2	1:4:176:LEU:HB2	2.55	0.41
1:D:113:GLU:HG2	1:D:131:MET:HE1	2.01	0.41
1:X:164:GLY:C	1:Y:170:HIS:CD2	2.93	0.41
1:1:117:ALA:O	1:1:121:GLY:N	2.54	0.41
1:4:173:TYR:OH	1:4:180:GLU:CD	2.59	0.41
1:4:191:VAL:O	1:4:191:VAL:HG23	2.20	0.41
1:4:138:THR:HA	1:5:138:THR:HA	2.03	0.41
1:C:92:VAL:N	2:C:205:HOH:O	2.52	0.41
1:5:117:ALA:CB	1:5:127:VAL:HG21	2.49	0.41
1:B:167:ASP:O	1:B:168:TYR:HB3	2.20	0.41
1:N:103:TRP:CZ3	1:N:156:MET:HG2	2.55	0.41
1:O:152:GLU:O	1:O:154:TYR:N	2.54	0.41
1:X:117:ALA:HB1	2:X:202:HOH:O	2.19	0.41
1:Z:138:THR:HG21	2:1:201:HOH:O	2.20	0.41
1:7:183:LYS:O	1:7:187:PHE:HB3	2.20	0.41
1:E:143:SER:HA	1:E:153:ALA:HB2	2.03	0.41
1:G:136:SER:HB2	1:H:138:THR:HG23	2.01	0.41
1:J:124:PRO:C	1:J:126:THR:H	2.23	0.41
1:P:158:ILE:O	1:P:158:ILE:HG13	2.21	0.41
1:Q:187:PHE:HA	1:Q:190:PHE:HD2	1.74	0.41
1:V:110:MET:HG2	1:V:116:VAL:HG13	2.02	0.41
1:2:116:VAL:O	1:2:121:GLY:N	2.53	0.41
1:4:103:TRP:CH2	1:4:156:MET:CG	3.04	0.41
1:O:176:LEU:HD12	1:O:181:LYS:HZ3	1.85	0.41
1:P:170:HIS:O	1:P:171:ARG:C	2.58	0.41
1:R:173:TYR:CE1	1:R:181:LYS:HG3	2.56	0.41
1:U:110:MET:HG3	1:U:116:VAL:HG22	2.03	0.41
1:W:185:THR:O	1:W:189:ASN:ND2	2.53	0.41
1:X:142:LEU:HA	1:X:145:LEU:HB2	2.02	0.41
1:Z:169:ASP:O	1:Z:172:MET:N	2.45	0.41
1:B:171:ARG:HG2	1:B:172:MET:N	2.36	0.41
1:C:176:LEU:HB3	1:C:180:GLU:CD	2.38	0.41
1:D:173:TYR:CE1	1:D:181:LYS:HG2	2.56	0.41
1:L:173:TYR:HA	1:L:176:LEU:HG	2.03	0.41
1:X:110:MET:HG3	1:X:111:THR:H	1.84	0.41
1:4:168:TYR:CE2	1:4:170:HIS:CD2	3.08	0.41
1:7:145:LEU:O	1:7:149:PHE:N	2.52	0.41
1:C:122:ILE:HG21	1:C:126:THR:HG21	2.03	0.41
1:M:172:MET:O	1:M:181:LYS:NZ	2.51	0.41
1:Z:139:ILE:HG21	1:1:142:LEU:HD23	2.03	0.41
1:4:93:GLU:HG3	1:5:139:ILE:HD11	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:190:PHE:CZ	1:5:190:PHE:HA	2.56	0.40
1:B:169:ASP:CG	1:B:172:MET:HG2	2.42	0.40
1:B:180:GLU:HA	1:B:183:LYS:HE2	2.02	0.40
1:F:187:PHE:CE1	1:F:191:VAL:HG11	2.56	0.40
1:U:142:LEU:HD23	1:U:153:ALA:HB1	2.03	0.40
1:V:113:GLU:OE2	1:V:125:ALA:HA	2.21	0.40
1:Z:176:LEU:HD12	1:Z:177:PRO:HD3	2.03	0.40
1:4:122:ILE:HG22	1:4:126:THR:OG1	2.20	0.40
1:6:176:LEU:HG	1:6:180:GLU:HG3	2.04	0.40
1:B:122:ILE:HG22	1:B:123:GLY:N	2.34	0.40
1:E:154:TYR:OH	1:F:165:ILE:HD11	2.21	0.40
1:M:182:ASN:C	1:M:184:ILE:N	2.74	0.40
1:N:165:ILE:HG22	1:N:166:ILE:H	1.84	0.40
1:N:192:PHE:O	1:N:193:GLU:CB	2.65	0.40
1:X:178:GLN:N	1:X:178:GLN:CD	2.74	0.40
1:Y:132:LYS:NZ	2:Y:204:HOH:O	2.53	0.40
1:Z:111:THR:HG22	1:Z:112:SER:H	1.87	0.40
1:3:100:LEU:HD22	1:3:130:ILE:HG22	2.03	0.40
1:3:165:ILE:HG23	1:3:166:ILE:N	2.36	0.40
1:3:188:ILE:O	1:3:191:VAL:HG23	2.21	0.40
1:4:92:VAL:HG13	1:4:93:GLU:N	2.37	0.40
1:5:171:ARG:CG	1:5:172:MET:N	2.77	0.40
1:6:181:LYS:HE2	1:7:166:ILE:HG21	2.04	0.40
1:B:184:ILE:O	1:B:188:ILE:HG12	2.21	0.40
1:C:107:ASP:HA	1:C:110:MET:HG2	2.02	0.40
1:H:189:ASN:CA	1:H:191:VAL:HG23	2.49	0.40
1:V:110:MET:HE3	1:V:112:SER:N	2.34	0.40
1:W:111:THR:HG21	2:W:208:HOH:O	2.21	0.40
1:1:130:ILE:CD1	1:1:141:VAL:HG11	2.51	0.40
1:1:95:GLN:OE1	1:1:159:PRO:HA	2.21	0.40
1:6:142:LEU:HD13	1:6:155:GLU:HG3	2.02	0.40
1:O:183:LYS:HA	1:O:186:SER:HB3	2.02	0.40
1:Q:146:ALA:HB2	1:Q:156:MET:CE	2.51	0.40
1:U:179:GLU:O	1:U:183:LYS:N	2.52	0.40
1:1:92:VAL:HG13	1:1:93:GLU:H	1.86	0.40
1:2:155:GLU:O	1:2:158:ILE:HG22	2.22	0.40
1:4:145:LEU:HD12	1:4:146:ALA:N	2.35	0.40
1:5:164:GLY:O	1:5:165:ILE:CB	2.70	0.40
1:F:162:ALA:N	1:F:163:PRO:CD	2.85	0.40
1:M:106:LYS:HG2	1:M:107:ASP:H	1.87	0.40
1:M:107:ASP:OD1	1:M:107:ASP:N	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:153:ALA:C	1:N:155:GLU:H	2.25	0.40
1:N:157:ILE:HG22	2:N:201:HOH:O	2.21	0.40
1:Z:173:TYR:O	1:Z:174:ALA:C	2.59	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:167:ASP:OD1	1:Y:111:THR:O[1_465]	2.04	0.16
1:I:133:ALA:O	1:L:147:ARG:NH1[1_455]	2.12	0.08

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1	103/107 (96%)	92 (89%)	9 (9%)	2 (2%)	9	37
1	2	99/107 (92%)	85 (86%)	13 (13%)	1 (1%)	17	54
1	3	98/107 (92%)	88 (90%)	6 (6%)	4 (4%)	3	16
1	4	98/107 (92%)	81 (83%)	15 (15%)	2 (2%)	8	35
1	5	98/107 (92%)	85 (87%)	10 (10%)	3 (3%)	4	23
1	6	99/107 (92%)	73 (74%)	17 (17%)	9 (9%)	1	3
1	7	103/107 (96%)	79 (77%)	19 (18%)	5 (5%)	2	13
1	A	103/107 (96%)	98 (95%)	5 (5%)	0	100	100
1	B	103/107 (96%)	95 (92%)	7 (7%)	1 (1%)	17	54
1	C	103/107 (96%)	95 (92%)	7 (7%)	1 (1%)	17	54
1	D	99/107 (92%)	93 (94%)	6 (6%)	0	100	100
1	E	103/107 (96%)	98 (95%)	5 (5%)	0	100	100
1	F	103/107 (96%)	101 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	G	103/107 (96%)	96 (93%)	7 (7%)	0	100	100
1	H	100/107 (94%)	94 (94%)	4 (4%)	2 (2%)	8	35
1	I	103/107 (96%)	87 (84%)	11 (11%)	5 (5%)	2	13
1	J	101/107 (94%)	89 (88%)	11 (11%)	1 (1%)	17	54
1	K	103/107 (96%)	84 (82%)	13 (13%)	6 (6%)	2	9
1	L	103/107 (96%)	90 (87%)	11 (11%)	2 (2%)	9	37
1	M	103/107 (96%)	80 (78%)	21 (20%)	2 (2%)	9	37
1	N	100/107 (94%)	85 (85%)	11 (11%)	4 (4%)	3	17
1	O	103/107 (96%)	86 (84%)	13 (13%)	4 (4%)	3	17
1	P	98/107 (92%)	82 (84%)	10 (10%)	6 (6%)	1	8
1	Q	103/107 (96%)	98 (95%)	5 (5%)	0	100	100
1	R	103/107 (96%)	99 (96%)	3 (3%)	1 (1%)	17	54
1	T	103/107 (96%)	97 (94%)	5 (5%)	1 (1%)	17	54
1	U	101/107 (94%)	98 (97%)	3 (3%)	0	100	100
1	V	103/107 (96%)	97 (94%)	6 (6%)	0	100	100
1	W	103/107 (96%)	100 (97%)	3 (3%)	0	100	100
1	X	103/107 (96%)	96 (93%)	6 (6%)	1 (1%)	17	54
1	Y	103/107 (96%)	90 (87%)	12 (12%)	1 (1%)	17	54
1	Z	98/107 (92%)	82 (84%)	13 (13%)	3 (3%)	4	23
All	All	3249/3424 (95%)	2893 (89%)	289 (9%)	67 (2%)	8	34

All (67) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	I	115	LYS
1	I	190	PHE
1	N	110	MET
1	N	165	ILE
1	P	112	SER
1	5	165	ILE
1	B	107	ASP
1	H	191	VAL
1	I	116	VAL
1	I	135	VAL
1	I	188	ILE

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Mol	Chain	Res	Type
1	K	153	ALA
1	K	160	VAL
1	N	172	MET
1	O	108	THR
1	O	109	GLU
1	O	153	ALA
1	O	155	GLU
1	P	111	THR
1	X	111	THR
1	Z	170	HIS
1	3	172	MET
1	4	160	VAL
1	5	174	ALA
1	6	133	ALA
1	7	110	MET
1	7	173	TYR
1	H	109	GLU
1	K	114	LYS
1	M	171	ARG
1	P	110	MET
1	P	190	PHE
1	R	111	THR
1	Z	190	PHE
1	1	160	VAL
1	3	162	ALA
1	6	96	ALA
1	6	98	ALA
1	6	108	THR
1	6	152	GLU
1	6	170	HIS
1	7	168	TYR
1	L	166	ILE
1	M	114	LYS
1	P	153	ALA
1	T	124	PRO
1	Z	127	VAL
1	3	123	GLY
1	3	173	TYR
1	5	172	MET
1	7	128	ASN
1	C	177	PRO
1	K	113	GLU

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Mol	Chain	Res	Type
1	K	133	ALA
1	L	107	ASP
1	N	143	SER
1	2	110	MET
1	6	163	PRO
1	6	177	PRO
1	6	191	VAL
1	Y	160	VAL
1	1	177	PRO
1	J	124	PRO
1	P	160	VAL
1	K	184	ILE
1	4	177	PRO
1	7	163	PRO

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1	84/86 (98%)	82 (98%)	2 (2%)	52	82
1	2	80/86 (93%)	75 (94%)	5 (6%)	20	53
1	3	79/86 (92%)	76 (96%)	3 (4%)	36	72
1	4	79/86 (92%)	75 (95%)	4 (5%)	26	62
1	5	79/86 (92%)	75 (95%)	4 (5%)	26	62
1	6	80/86 (93%)	73 (91%)	7 (9%)	11	37
1	7	84/86 (98%)	80 (95%)	4 (5%)	28	65
1	A	84/86 (98%)	81 (96%)	3 (4%)	38	73
1	B	84/86 (98%)	80 (95%)	4 (5%)	28	65
1	C	84/86 (98%)	77 (92%)	7 (8%)	12	40
1	D	80/86 (93%)	78 (98%)	2 (2%)	50	81
1	E	84/86 (98%)	82 (98%)	2 (2%)	52	82
1	F	84/86 (98%)	84 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	84/86 (98%)	79 (94%)	5 (6%)	21	56
1	H	81/86 (94%)	79 (98%)	2 (2%)	50	81
1	I	84/86 (98%)	80 (95%)	4 (5%)	28	65
1	J	82/86 (95%)	77 (94%)	5 (6%)	20	55
1	K	84/86 (98%)	79 (94%)	5 (6%)	21	56
1	L	84/86 (98%)	78 (93%)	6 (7%)	16	48
1	M	84/86 (98%)	75 (89%)	9 (11%)	7	27
1	N	81/86 (94%)	76 (94%)	5 (6%)	20	54
1	O	84/86 (98%)	76 (90%)	8 (10%)	9	33
1	P	79/86 (92%)	75 (95%)	4 (5%)	26	62
1	Q	84/86 (98%)	80 (95%)	4 (5%)	28	65
1	R	84/86 (98%)	82 (98%)	2 (2%)	52	82
1	T	84/86 (98%)	81 (96%)	3 (4%)	38	73
1	U	82/86 (95%)	80 (98%)	2 (2%)	52	82
1	V	84/86 (98%)	83 (99%)	1 (1%)	74	91
1	W	84/86 (98%)	82 (98%)	2 (2%)	52	82
1	X	84/86 (98%)	78 (93%)	6 (7%)	16	48
1	Y	84/86 (98%)	82 (98%)	2 (2%)	52	82
1	Z	79/86 (92%)	71 (90%)	8 (10%)	8	30
All	All	2641/2752 (96%)	2511 (95%)	130 (5%)	27	64

All (130) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	113	GLU
1	A	136	SER
1	A	193	GLU
1	B	105	ARG
1	B	171	ARG
1	B	182	ASN
1	B	185	THR
1	C	99	THR
1	C	114	LYS
1	C	115	LYS
1	C	122	ILE

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Mol	Chain	Res	Type
1	C	176	LEU
1	C	180	GLU
1	C	195	ASN
1	D	170	HIS
1	D	185	THR
1	E	138	THR
1	E	167	ASP
1	G	110	MET
1	G	111	THR
1	G	127	VAL
1	G	147	ARG
1	G	149	PHE
1	H	171	ARG
1	H	178	GLN
1	I	114	LYS
1	I	115	LYS
1	I	127	VAL
1	I	178	GLN
1	J	95	GLN
1	J	110	MET
1	J	142	LEU
1	J	154	TYR
1	J	176	LEU
1	K	105	ARG
1	K	114	LYS
1	K	130	ILE
1	K	132	LYS
1	K	189	ASN
1	L	93	GLU
1	L	138	THR
1	L	145	LEU
1	L	152	GLU
1	L	179	GLU
1	L	193	GLU
1	M	94	LYS
1	M	107	ASP
1	M	110	MET
1	M	118	VAL
1	M	128	ASN
1	M	173	TYR
1	M	176	LEU
1	M	182	ASN

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Mol	Chain	Res	Type
1	M	192	PHE
1	N	113	GLU
1	N	151	HIS
1	N	171	ARG
1	N	176	LEU
1	N	178	GLN
1	O	94	LYS
1	O	109	GLU
1	O	151	HIS
1	O	152	GLU
1	O	170	HIS
1	O	171	ARG
1	O	190	PHE
1	O	194	GLN
1	P	93	GLU
1	P	110	MET
1	P	111	THR
1	P	115	LYS
1	Q	92	VAL
1	Q	157	ILE
1	Q	176	LEU
1	Q	180	GLU
1	R	136	SER
1	R	167	ASP
1	T	101	ASN
1	T	111	THR
1	T	136	SER
1	U	107	ASP
1	U	178	GLN
1	V	115	LYS
1	W	178	GLN
1	W	185	THR
1	X	110	MET
1	X	111	THR
1	X	115	LYS
1	X	166	ILE
1	X	172	MET
1	X	196	LYS
1	Y	94	LYS
1	Y	176	LEU
1	Z	111	THR
1	Z	129	ARG

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Mol	Chain	Res	Type
1	Z	134	GLU
1	Z	156	MET
1	Z	158	ILE
1	Z	167	ASP
1	Z	184	ILE
1	Z	191	VAL
1	1	107	ASP
1	1	179	GLU
1	2	100	LEU
1	2	105	ARG
1	2	110	MET
1	2	122	ILE
1	2	135	VAL
1	3	122	ILE
1	3	141	VAL
1	3	172	MET
1	4	104	MET
1	4	129	ARG
1	4	170	HIS
1	4	190	PHE
1	5	130	ILE
1	5	171	ARG
1	5	172	MET
1	5	173	TYR
1	6	92	VAL
1	6	132	LYS
1	6	136	SER
1	6	147	ARG
1	6	156	MET
1	6	169	ASP
1	6	170	HIS
1	7	101	ASN
1	7	106	LYS
1	7	122	ILE
1	7	170	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	101	ASN
1	G	128	ASN
1	G	151	HIS

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Mol	Chain	Res	Type
1	G	194	GLN
1	I	178	GLN
1	J	182	ASN
1	K	189	ASN
1	O	95	GLN
1	O	128	ASN
1	O	151	HIS
1	O	170	HIS
1	O	195	ASN
1	Q	182	ASN
1	R	194	GLN
1	T	182	ASN
1	T	195	ASN
1	U	182	ASN
1	W	101	ASN
1	X	195	ASN
1	Y	195	ASN
1	Z	95	GLN
1	Z	178	GLN
1	Z	182	ASN
1	2	182	ASN
1	4	95	GLN
1	4	128	ASN
1	5	170	HIS
1	6	170	HIS
1	7	101	ASN
1	7	170	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

There are no ligands in this entry.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	1	105/107 (98%)	0.12	3 (2%) 51 31	47, 87, 110, 116	0
1	2	101/107 (94%)	0.47	9 (8%) 9 5	61, 99, 133, 140	0
1	3	100/107 (93%)	0.20	2 (2%) 65 44	41, 83, 111, 139	0
1	4	100/107 (93%)	0.66	18 (18%) 1 0	64, 100, 138, 150	0
1	5	100/107 (93%)	0.40	7 (7%) 16 8	54, 94, 122, 139	0
1	6	101/107 (94%)	0.92	18 (17%) 1 1	55, 111, 136, 154	0
1	7	105/107 (98%)	0.53	15 (14%) 2 1	63, 99, 124, 129	0
1	A	105/107 (98%)	-0.07	2 (1%) 66 46	33, 64, 96, 105	0
1	B	105/107 (98%)	-0.01	1 (0%) 82 65	31, 54, 87, 99	0
1	C	105/107 (98%)	-0.08	2 (1%) 66 46	34, 60, 92, 117	0
1	D	101/107 (94%)	-0.20	0 100 100	33, 49, 69, 79	0
1	E	105/107 (98%)	-0.16	0 100 100	37, 60, 84, 102	0
1	F	105/107 (98%)	-0.26	2 (1%) 66 46	24, 46, 72, 83	0
1	G	105/107 (98%)	-0.17	1 (0%) 82 65	35, 63, 116, 127	0
1	H	102/107 (95%)	-0.20	1 (0%) 82 65	30, 52, 76, 85	0
1	I	105/107 (98%)	0.52	7 (6%) 18 9	60, 100, 126, 137	0
1	J	103/107 (96%)	0.13	2 (1%) 66 46	62, 89, 121, 134	0
1	K	105/107 (98%)	0.48	11 (10%) 6 3	69, 105, 132, 158	0
1	L	105/107 (98%)	0.31	4 (3%) 40 23	61, 85, 115, 118	0
1	M	105/107 (98%)	0.53	9 (8%) 10 5	75, 105, 142, 168	0
1	N	102/107 (95%)	0.36	7 (6%) 17 9	52, 92, 119, 125	0
1	O	105/107 (98%)	0.62	14 (13%) 3 1	66, 106, 123, 131	0
1	P	100/107 (93%)	0.38	8 (8%) 12 6	59, 91, 120, 133	0
1	Q	105/107 (98%)	0.06	5 (4%) 30 17	34, 64, 94, 104	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	R	105/107 (98%)	-0.03	1 (0%) 82 65	32, 53, 80, 106	0
1	T	105/107 (98%)	0.01	2 (1%) 66 46	41, 58, 100, 118	0
1	U	103/107 (96%)	-0.25	0 100 100	29, 42, 64, 74	0
1	V	105/107 (98%)	-0.08	1 (0%) 82 65	40, 65, 89, 110	0
1	W	105/107 (98%)	-0.19	2 (1%) 66 46	27, 45, 80, 97	0
1	X	105/107 (98%)	-0.10	2 (1%) 66 46	38, 68, 111, 117	0
1	Y	105/107 (98%)	-0.05	3 (2%) 51 31	32, 58, 95, 128	0
1	Z	100/107 (93%)	0.56	14 (14%) 2 1	64, 104, 132, 140	0
All	All	3313/3424 (96%)	0.17	173 (5%) 27 15	24, 77, 122, 168	0

All (173) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	4	102	ALA	7.7
1	K	117	ALA	7.1
1	O	92	VAL	6.4
1	M	195	ASN	5.9
1	6	160	VAL	5.5
1	6	161	GLY	5.4
1	C	111	THR	5.4
1	P	184	ILE	5.4
1	P	185	THR	5.2
1	Z	102	ALA	4.6
1	O	94	LYS	4.6
1	5	110	MET	4.5
1	Z	161	GLY	4.5
1	6	149	PHE	4.3
1	6	163	PRO	4.3
1	6	102	ALA	4.1
1	O	112	SER	4.0
1	4	159	PRO	4.0
1	6	128	ASN	4.0
1	Z	103	TRP	3.9
1	7	137	THR	3.9
1	2	128	ASN	3.8
1	7	177	PRO	3.8
1	4	96	ALA	3.8
1	N	130	ILE	3.7
1	K	102	ALA	3.7

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Mol	Chain	Res	Type	RSRZ
1	6	98	ALA	3.6
1	K	195	ASN	3.6
1	7	178	GLN	3.6
1	R	111	THR	3.6
1	7	150	GLY	3.5
1	M	159	PRO	3.5
1	2	185	THR	3.4
1	7	148	ALA	3.4
1	K	156	MET	3.4
1	X	118	VAL	3.4
1	Z	168	TYR	3.4
1	C	108	THR	3.4
1	1	164	GLY	3.3
1	Z	107	ASP	3.3
1	Y	193	GLU	3.3
1	K	132	LYS	3.3
1	Z	185	THR	3.3
1	7	119	ALA	3.3
1	7	111	THR	3.2
1	4	115	LYS	3.2
1	4	154	TYR	3.2
1	I	124	PRO	3.2
1	4	98	ALA	3.2
1	6	105	ARG	3.2
1	2	111	THR	3.2
1	4	131	MET	3.2
1	4	176	LEU	3.1
1	B	111	THR	3.1
1	Z	162	ALA	3.1
1	4	178	GLN	3.1
1	Z	125	ALA	3.1
1	4	114	LYS	3.0
1	P	112	SER	3.0
1	M	138	THR	3.0
1	6	190	PHE	2.9
1	O	146	ALA	2.9
1	2	108	THR	2.9
1	Q	111	THR	2.9
1	2	134	GLU	2.9
1	N	127	VAL	2.9
1	2	98	ALA	2.8
1	O	157	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
1	M	128	ASN	2.8
1	O	175	ALA	2.8
1	4	105	ARG	2.8
1	4	94	LYS	2.8
1	I	104	MET	2.8
1	O	103	TRP	2.8
1	5	92	VAL	2.8
1	M	102	ALA	2.8
1	I	112	SER	2.7
1	6	107	ASP	2.7
1	M	174	ALA	2.7
1	2	168	TYR	2.7
1	W	190	PHE	2.7
1	K	96	ALA	2.7
1	L	175	ALA	2.7
1	K	126	THR	2.7
1	4	138	THR	2.7
1	N	171	ARG	2.7
1	6	133	ALA	2.7
1	M	118	VAL	2.7
1	4	95	GLN	2.7
1	7	92	VAL	2.7
1	P	125	ALA	2.7
1	Q	188	ILE	2.6
1	L	110	MET	2.6
1	Z	112	SER	2.6
1	5	108	THR	2.6
1	M	137	THR	2.6
1	I	194	GLN	2.6
1	O	187	PHE	2.6
1	A	111	THR	2.6
1	V	111	THR	2.6
1	Q	121	GLY	2.6
1	2	160	VAL	2.5
1	Q	120	ALA	2.5
1	6	162	ALA	2.5
1	T	124	PRO	2.5
1	5	146	ALA	2.5
1	6	148	ALA	2.5
1	H	111	THR	2.5
1	K	103	TRP	2.5
1	7	118	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	3	110	MET	2.5
1	I	188	ILE	2.5
1	Z	117	ALA	2.5
1	A	194	GLN	2.5
1	I	151	HIS	2.5
1	K	129	ARG	2.4
1	7	113	GLU	2.4
1	P	186	SER	2.4
1	N	110	MET	2.4
1	5	168	TYR	2.4
1	T	110	MET	2.4
1	Y	176	LEU	2.4
1	Q	118	VAL	2.4
1	F	166	ILE	2.4
1	O	171	ARG	2.4
1	7	99	THR	2.3
1	2	110	MET	2.3
1	I	195	ASN	2.3
1	O	133	ALA	2.3
1	7	149	PHE	2.3
1	J	110	MET	2.3
1	M	103	TRP	2.3
1	K	157	ILE	2.3
1	1	128	ASN	2.3
1	Y	191	VAL	2.3
1	1	110	MET	2.3
1	W	194	GLN	2.3
1	P	180	GLU	2.3
1	Z	108	THR	2.3
1	6	108	THR	2.3
1	O	170	HIS	2.3
1	N	137	THR	2.2
1	J	170	HIS	2.2
1	L	136	SER	2.2
1	6	136	SER	2.2
1	Z	126	THR	2.2
1	G	193	GLU	2.2
1	4	99	THR	2.2
1	6	106	LYS	2.2
1	O	142	LEU	2.2
1	N	121	GLY	2.2
1	4	165	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	N	151	HIS	2.2
1	P	144	SER	2.1
1	5	127	VAL	2.1
1	3	174	ALA	2.1
1	O	189	ASN	2.1
1	5	145	LEU	2.1
1	L	103	TRP	2.1
1	Z	156	MET	2.1
1	4	111	THR	2.1
1	P	168	TYR	2.1
1	4	101	ASN	2.1
1	O	93	GLU	2.1
1	7	141	VAL	2.1
1	6	103	TRP	2.1
1	F	187	PHE	2.1
1	X	185	THR	2.0
1	Z	111	THR	2.0
1	7	98	ALA	2.0
1	6	166	ILE	2.0
1	7	136	SER	2.0
1	K	131	MET	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.