



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:20 AM GMT

PDB ID : 2Q4H  
Title : Ensemble refinement of the crystal structure of GALT-like protein from *Arabidopsis thaliana* At5g18200  
Authors : Levin, E.J.; Kondrashov, D.A.; Wesenberg, G.E.; Phillips Jr., G.N.; Center for Eukaryotic Structural Genomics (CESG)  
Deposited on : 2007-05-31  
Resolution : 1.83 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

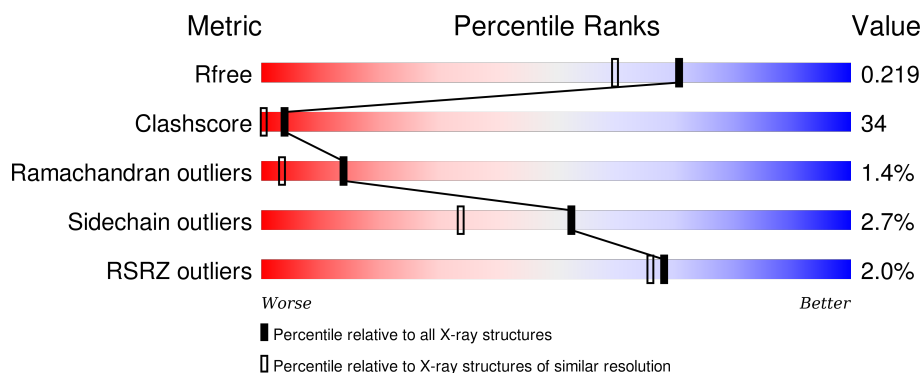
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.83 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))
$R_{free}$	91344	2634 (1.86-1.82)
Clashscore	102246	2862 (1.86-1.82)
Ramachandran outliers	100387	2831 (1.86-1.82)
Sidechain outliers	100360	2832 (1.86-1.82)
RSRZ outliers	91569	2639 (1.86-1.82)

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-A	351	<div> <div>2%</div> <div>46%</div> <div>41%</div> <div>•</div> <div>11%</div> </div>
1	1-B	351	<div> <div>2%</div> <div>41%</div> <div>42%</div> <div>•</div> <div>13%</div> </div>
1	2-A	351	<div> <div>2%</div> <div>47%</div> <div>39%</div> <div>•</div> <div>11%</div> </div>
1	2-B	351	<div> <div>2%</div> <div>48%</div> <div>36%</div> <div>•</div> <div>13%</div> </div>
1	3-A	351	<div> <div>2%</div> <div>42%</div> <div>44%</div> <div>•</div> <div>11%</div> </div>

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Mol	Chain	Length	Quality of chain
1	3-B	351	
1	4-A	351	
1	4-B	351	
1	5-A	351	
1	5-B	351	
1	6-A	351	
1	6-B	351	
1	7-A	351	
1	7-B	351	
1	8-A	351	
1	8-B	351	

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
2	ZN	1-A	604	-	-	-	X
2	ZN	2-A	604	-	-	-	X
2	ZN	3-A	604	-	-	-	X
2	ZN	4-A	604	-	-	-	X
2	ZN	6-A	604	-	-	-	X
2	ZN	7-A	604	-	-	-	X
3	AMP	1-A	601	-	-	X	-
3	AMP	2-A	601	-	-	X	-
3	AMP	6-B	602	-	-	X	-
4	EDO	1-A	608	-	-	-	X
4	EDO	1-A	609	-	-	-	X
4	EDO	1-B	610	-	-	-	X
4	EDO	1-B	611	-	-	-	X
4	EDO	1-B	612	-	-	-	X
4	EDO	2-A	608	-	-	-	X
4	EDO	2-A	609	-	-	-	X
4	EDO	2-B	610	-	-	-	X
4	EDO	2-B	611	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	EDO	2-B	612	-	-	-	X
4	EDO	3-A	608	-	-	-	X
4	EDO	3-A	609	-	-	-	X
4	EDO	3-B	610	-	-	X	X
4	EDO	3-B	611	-	-	-	X
4	EDO	3-B	612	-	-	-	X
4	EDO	4-A	608	-	-	-	X
4	EDO	4-A	609	-	-	-	X
4	EDO	4-B	610	-	-	-	X
4	EDO	4-B	611	-	-	-	X
4	EDO	4-B	612	-	-	-	X
4	EDO	5-A	608	-	-	-	X
4	EDO	5-A	609	-	-	-	X
4	EDO	5-B	610	-	-	-	X
4	EDO	5-B	611	-	-	-	X
4	EDO	5-B	612	-	-	-	X
4	EDO	6-A	608	-	-	-	X
4	EDO	6-A	609	-	-	-	X
4	EDO	6-B	610	-	-	-	X
4	EDO	6-B	611	-	-	-	X
4	EDO	6-B	612	-	-	-	X
4	EDO	7-A	608	-	-	-	X
4	EDO	7-A	609	-	-	-	X
4	EDO	7-B	610	-	-	-	X
4	EDO	7-B	611	-	-	-	X
4	EDO	7-B	612	-	-	-	X
4	EDO	8-A	607	-	-	X	-
4	EDO	8-A	608	-	-	-	X
4	EDO	8-A	609	-	-	-	X
4	EDO	8-B	610	-	-	-	X
4	EDO	8-B	611	-	-	-	X
4	EDO	8-B	612	-	-	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 43592 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.

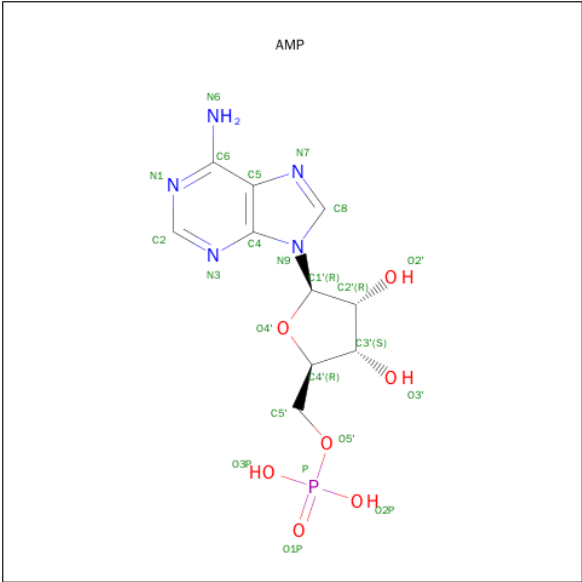
- Molecule 1 is a protein called Probable galactose-1-phosphate uridyl transferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1-A	311	Total	C	N	O	S	0	0	0
			2461	1577	417	454	13			
1	2-A	311	Total	C	N	O	S	0	0	0
			2461	1577	417	454	13			
1	3-A	311	Total	C	N	O	S	0	0	0
			2461	1577	417	454	13			
1	4-A	311	Total	C	N	O	S	0	0	0
			2461	1577	417	454	13			
1	5-A	311	Total	C	N	O	S	0	0	0
			2461	1577	417	454	13			
1	6-A	311	Total	C	N	O	S	0	0	0
			2461	1577	417	454	13			
1	7-A	311	Total	C	N	O	S	0	0	0
			2461	1577	417	454	13			
1	8-A	311	Total	C	N	O	S	0	0	0
			2461	1577	417	454	13			
1	1-B	305	Total	C	N	O	S	0	0	0
			2416	1550	408	445	13			
1	2-B	305	Total	C	N	O	S	0	0	0
			2416	1550	408	445	13			
1	3-B	305	Total	C	N	O	S	0	0	0
			2416	1550	408	445	13			
1	4-B	305	Total	C	N	O	S	0	0	0
			2416	1550	408	445	13			
1	5-B	305	Total	C	N	O	S	0	0	0
			2416	1550	408	445	13			
1	6-B	305	Total	C	N	O	S	0	0	0
			2416	1550	408	445	13			
1	7-B	305	Total	C	N	O	S	0	0	0
			2416	1550	408	445	13			
1	8-B	305	Total	C	N	O	S	0	0	0
			2416	1550	408	445	13			

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	7-B	2	Total 2	Zn 2	0	0
2	3-A	2	Total 2	Zn 2	0	0
2	8-B	2	Total 2	Zn 2	0	0
2	3-B	2	Total 2	Zn 2	0	0
2	5-B	2	Total 2	Zn 2	0	0
2	4-A	2	Total 2	Zn 2	0	0
2	1-B	2	Total 2	Zn 2	0	0
2	5-A	2	Total 2	Zn 2	0	0
2	6-B	2	Total 2	Zn 2	0	0
2	8-A	2	Total 2	Zn 2	0	0
2	1-A	2	Total 2	Zn 2	0	0
2	6-A	2	Total 2	Zn 2	0	0
2	2-B	2	Total 2	Zn 2	0	0
2	2-A	2	Total 2	Zn 2	0	0
2	4-B	2	Total 2	Zn 2	0	0
2	7-A	2	Total 2	Zn 2	0	0

- Molecule 3 is ADENOSINE MONOPHOSPHATE (three-letter code: AMP) (formula: C<sub>10</sub>H<sub>14</sub>N<sub>5</sub>O<sub>7</sub>P).



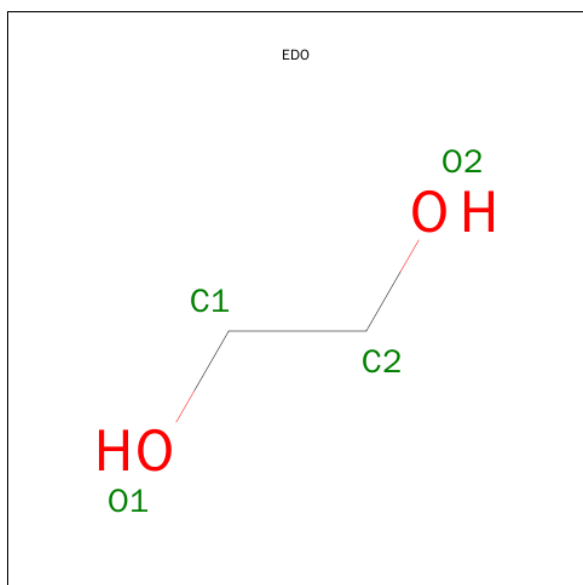
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	1-A	1	Total	C	N	O	P	0	0
			22	10	5	6	1		
3	2-A	1	Total	C	N	O	P	0	0
			22	10	5	6	1		
3	3-A	1	Total	C	N	O	P	0	0
			22	10	5	6	1		
3	4-A	1	Total	C	N	O	P	0	0
			22	10	5	6	1		
3	5-A	1	Total	C	N	O	P	0	0
			22	10	5	6	1		
3	6-A	1	Total	C	N	O	P	0	0
			22	10	5	6	1		
3	7-A	1	Total	C	N	O	P	0	0
			22	10	5	6	1		
3	8-A	1	Total	C	N	O	P	0	0
			22	10	5	6	1		
3	1-B	1	Total	C	N	O	P	0	0
			22	10	5	6	1		
3	2-B	1	Total	C	N	O	P	0	0
			22	10	5	6	1		
3	3-B	1	Total	C	N	O	P	0	0
			22	10	5	6	1		
3	4-B	1	Total	C	N	O	P	0	0
			22	10	5	6	1		
3	5-B	1	Total	C	N	O	P	0	0
			22	10	5	6	1		
3	6-B	1	Total	C	N	O	P	0	0
			22	10	5	6	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	7-B	1	Total	C	N	O	P	0	0
			22	10	5	6	1		
3	8-B	1	Total	C	N	O	P	0	0
			22	10	5	6	1		

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	1-A	1	Total	C	O	0	0
			4	2	2		
4	2-A	1	Total	C	O	0	0
			4	2	2		
4	3-A	1	Total	C	O	0	0
			4	2	2		
4	4-A	1	Total	C	O	0	0
			4	2	2		
4	5-A	1	Total	C	O	0	0
			4	2	2		
4	6-A	1	Total	C	O	0	0
			4	2	2		
4	7-A	1	Total	C	O	0	0
			4	2	2		
4	8-A	1	Total	C	O	0	0
			4	2	2		
4	1-A	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	2-A	1	Total 4	C 2	O 2	0	0
4	3-A	1	Total 4	C 2	O 2	0	0
4	4-A	1	Total 4	C 2	O 2	0	0
4	5-A	1	Total 4	C 2	O 2	0	0
4	6-A	1	Total 4	C 2	O 2	0	0
4	7-A	1	Total 4	C 2	O 2	0	0
4	8-A	1	Total 4	C 2	O 2	0	0
4	1-A	1	Total 4	C 2	O 2	0	0
4	2-A	1	Total 4	C 2	O 2	0	0
4	3-A	1	Total 4	C 2	O 2	0	0
4	4-A	1	Total 4	C 2	O 2	0	0
4	5-A	1	Total 4	C 2	O 2	0	0
4	6-A	1	Total 4	C 2	O 2	0	0
4	7-A	1	Total 4	C 2	O 2	0	0
4	8-A	1	Total 4	C 2	O 2	0	0
4	1-B	1	Total 4	C 2	O 2	0	0
4	2-B	1	Total 4	C 2	O 2	0	0
4	3-B	1	Total 4	C 2	O 2	0	0
4	4-B	1	Total 4	C 2	O 2	0	0
4	5-B	1	Total 4	C 2	O 2	0	0
4	6-B	1	Total 4	C 2	O 2	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	7-B	1	Total	C	O	0	0
			4	2	2		
4	8-B	1	Total	C	O	0	0
			4	2	2		
4	1-B	1	Total	C	O	0	0
			4	2	2		
4	2-B	1	Total	C	O	0	0
			4	2	2		
4	3-B	1	Total	C	O	0	0
			4	2	2		
4	4-B	1	Total	C	O	0	0
			4	2	2		
4	5-B	1	Total	C	O	0	0
			4	2	2		
4	6-B	1	Total	C	O	0	0
			4	2	2		
4	7-B	1	Total	C	O	0	0
			4	2	2		
4	8-B	1	Total	C	O	0	0
			4	2	2		
4	1-B	1	Total	C	O	0	0
			4	2	2		
4	2-B	1	Total	C	O	0	0
			4	2	2		
4	3-B	1	Total	C	O	0	0
			4	2	2		
4	4-B	1	Total	C	O	0	0
			4	2	2		
4	5-B	1	Total	C	O	0	0
			4	2	2		
4	6-B	1	Total	C	O	0	0
			4	2	2		
4	7-B	1	Total	C	O	0	0
			4	2	2		
4	8-B	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	1-A	273	Total	O	0	0
			273	273		

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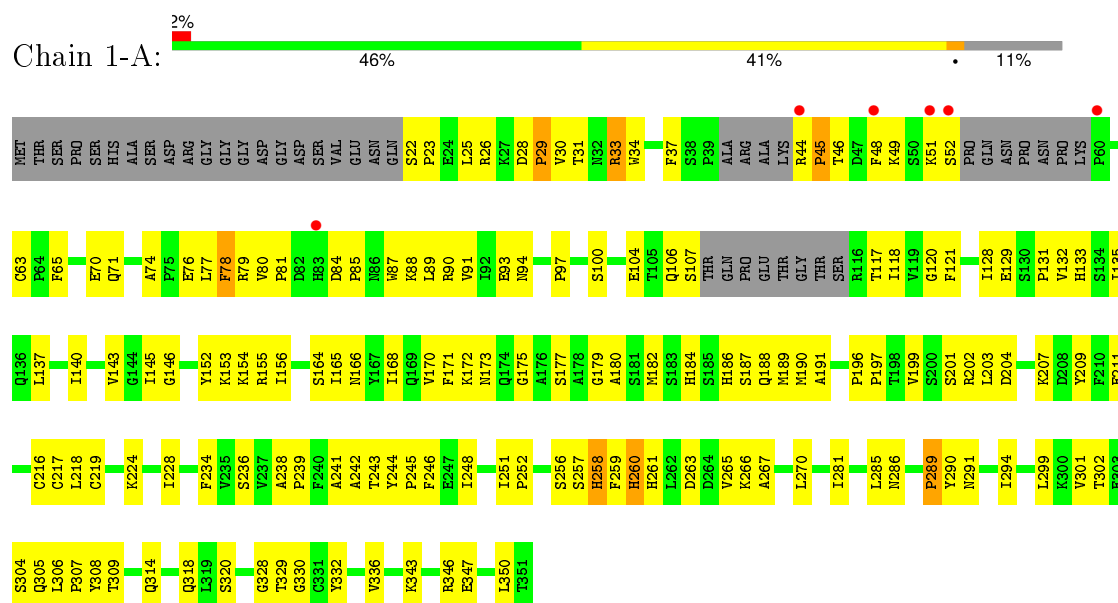
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	2-A	274	Total 274	O 274	0	0
5	3-A	270	Total 270	O 270	0	0
5	4-A	272	Total 272	O 272	0	0
5	5-A	270	Total 270	O 270	0	0
5	6-A	270	Total 270	O 270	0	0
5	7-A	270	Total 270	O 270	0	0
5	8-A	271	Total 271	O 271	0	0
5	1-B	227	Total 227	O 227	0	0
5	2-B	226	Total 226	O 226	0	0
5	3-B	230	Total 230	O 230	0	0
5	4-B	228	Total 228	O 228	0	0
5	5-B	230	Total 230	O 230	0	0
5	6-B	230	Total 230	O 230	0	0
5	7-B	230	Total 230	O 230	0	0
5	8-B	229	Total 229	O 229	0	0

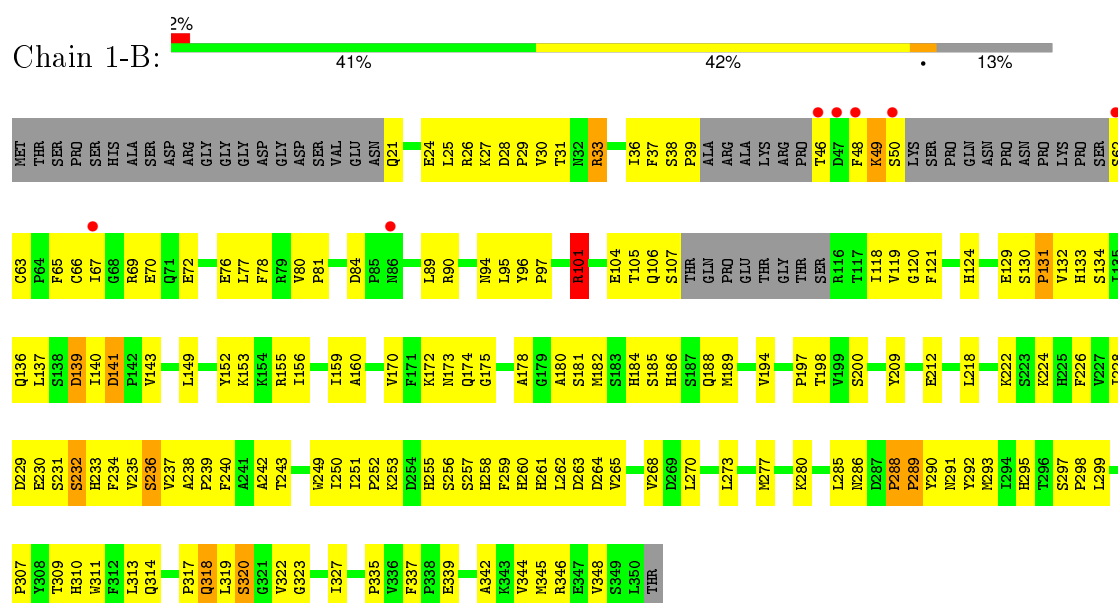
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

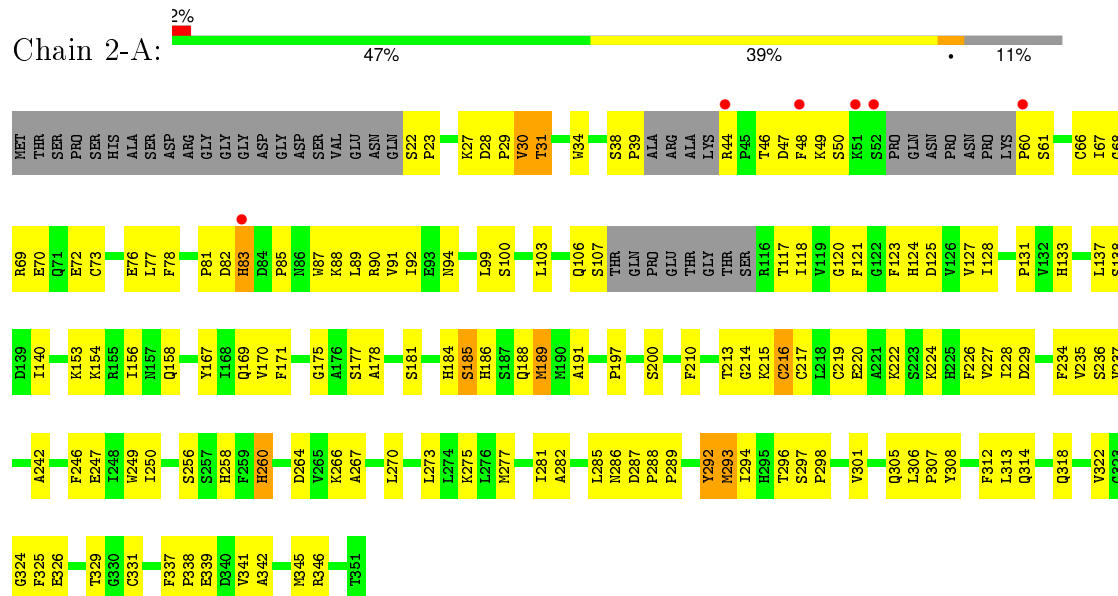
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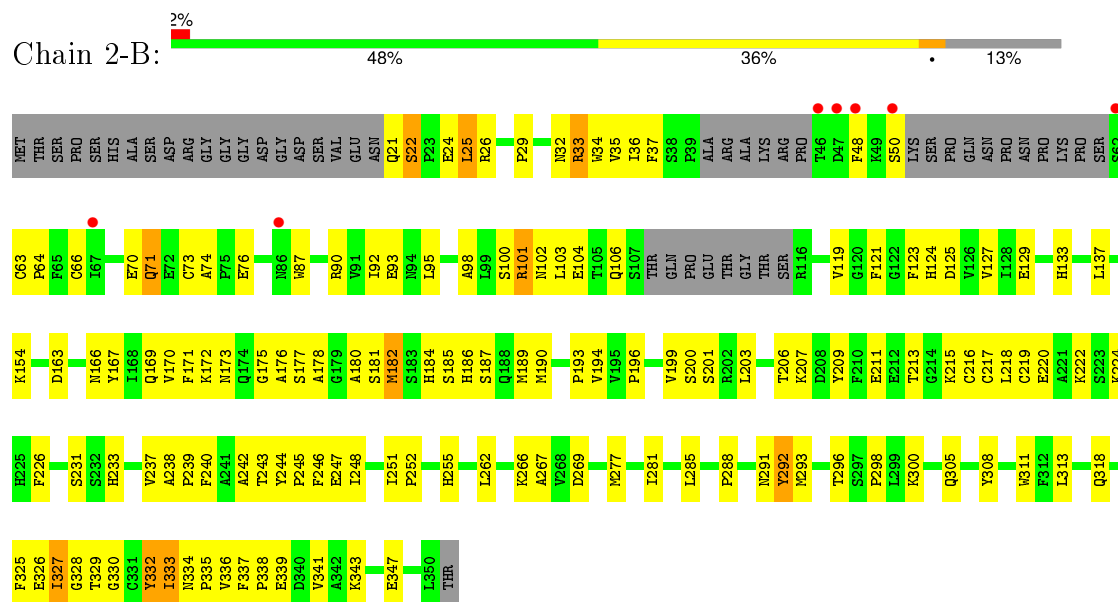
- Molecule 1: Probable galactose-1-phosphate uridyl transferase



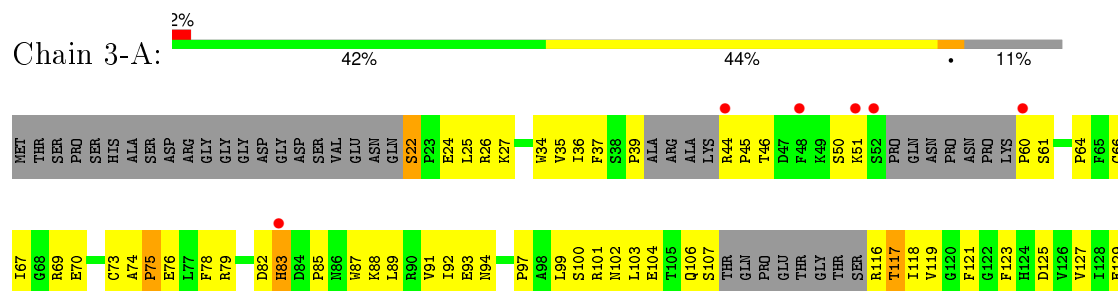
- Molecule 1: Probable galactose-1-phosphate uridyl transferase

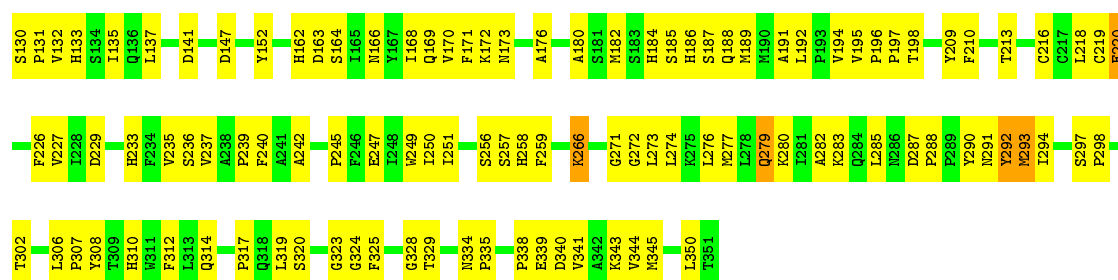


- Molecule 1: Probable galactose-1-phosphate uridyl transferase

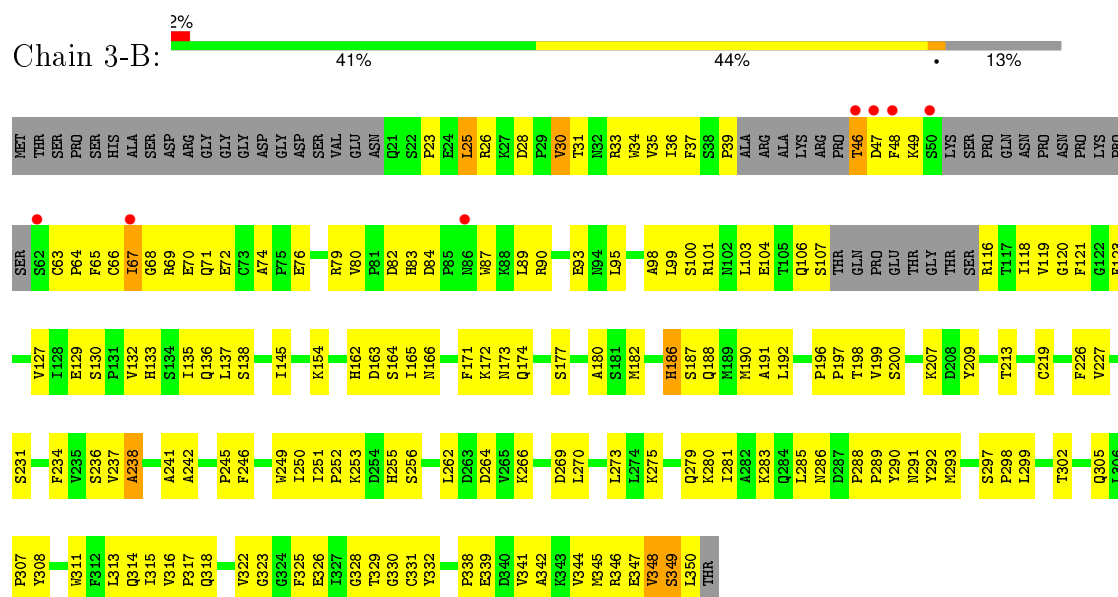


- Molecule 1: Probable galactose-1-phosphate uridyl transferase

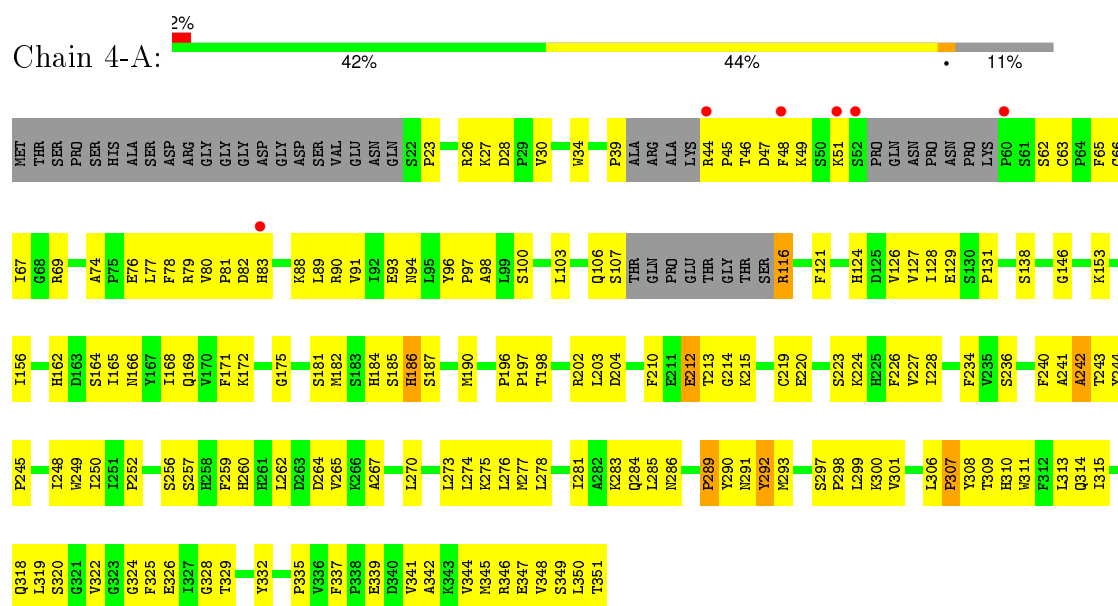




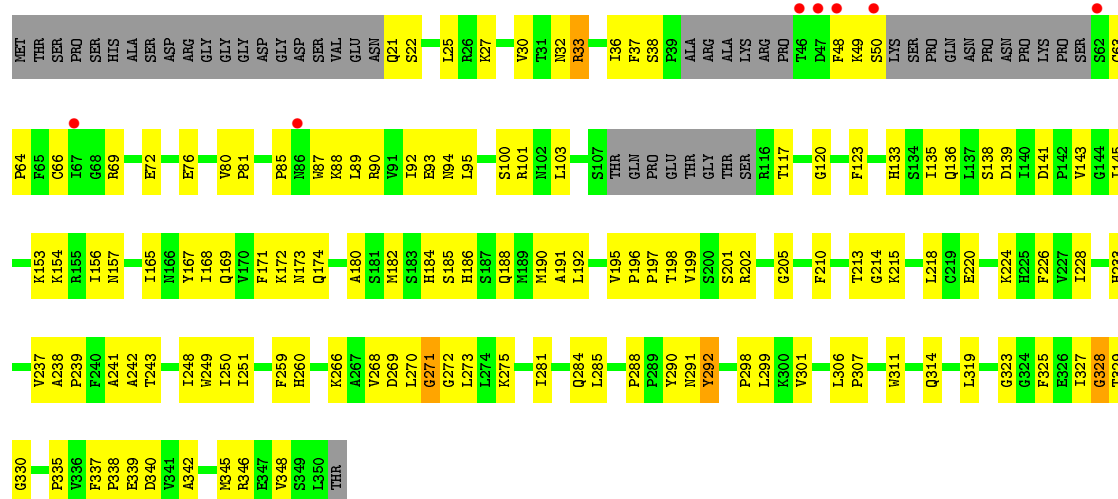
- Molecule 1: Probable galactose-1-phosphate uridyl transferase



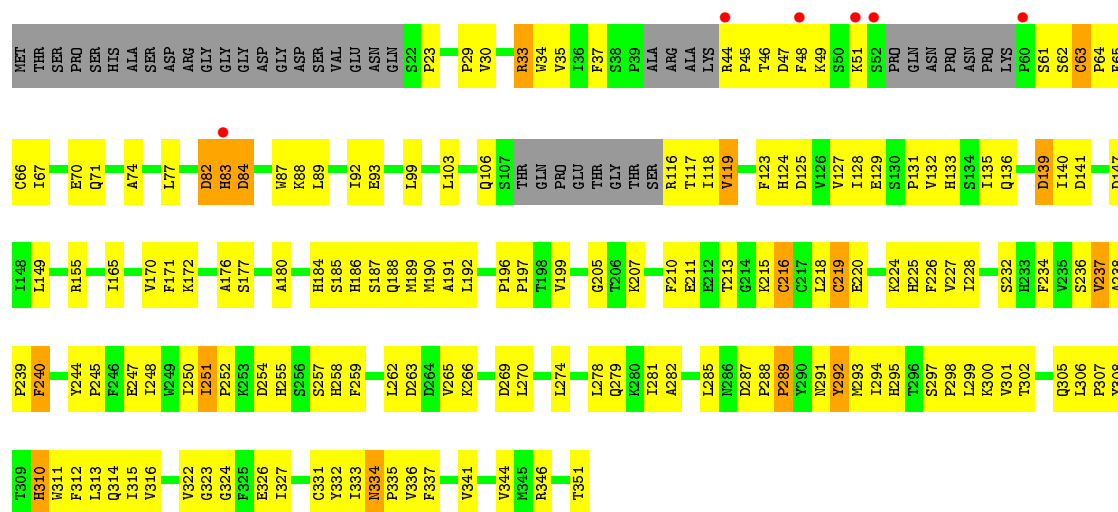
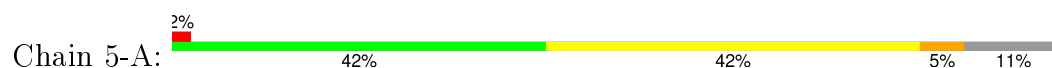
- Molecule 1: Probable galactose-1-phosphate uridyl transferase



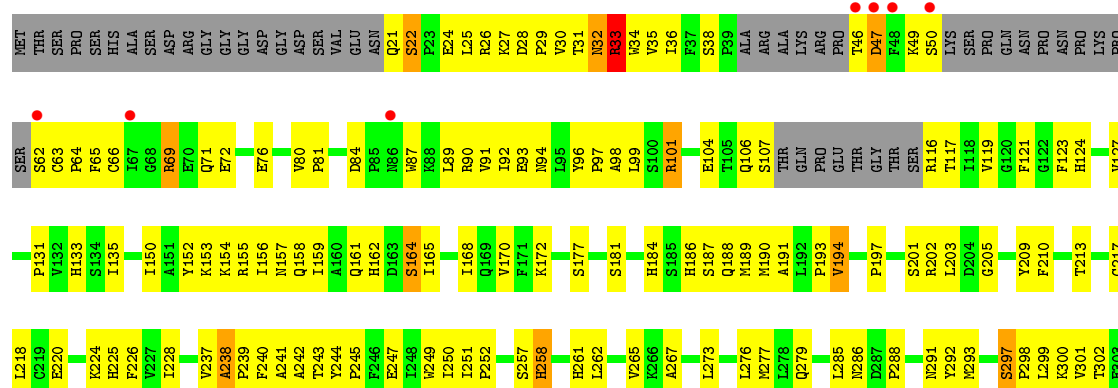
- Molecule 1: Probable galactose-1-phosphate uridyl transferase



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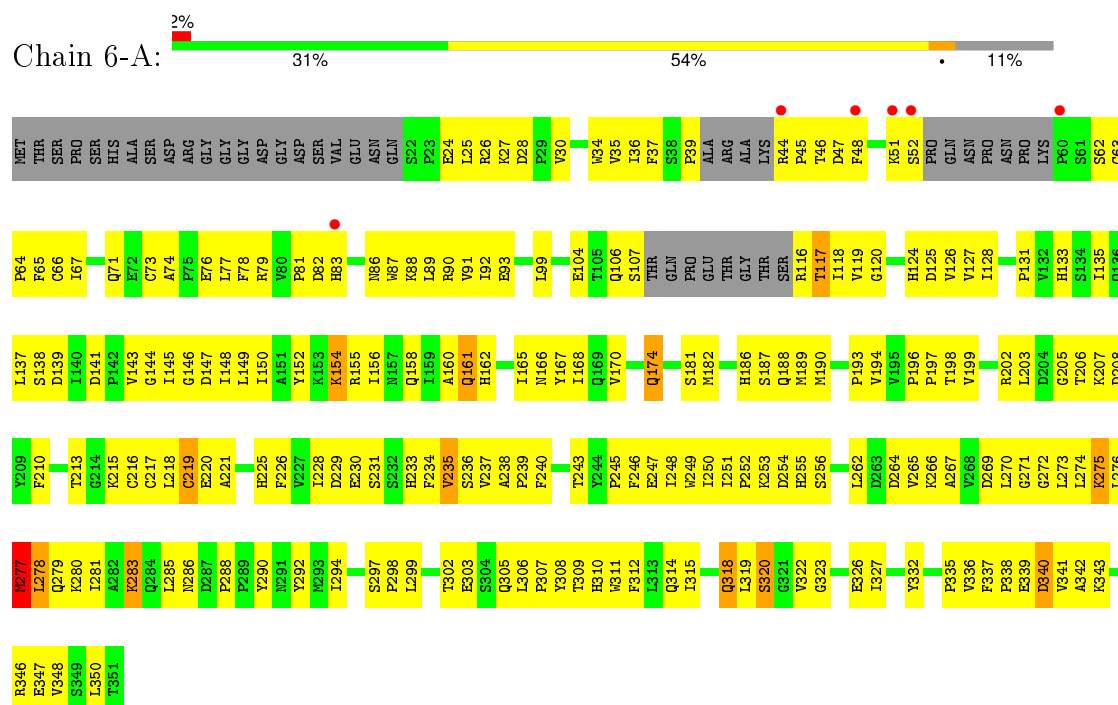


- Molecule 1: Probable galactose-1-phosphate uridyl transferase

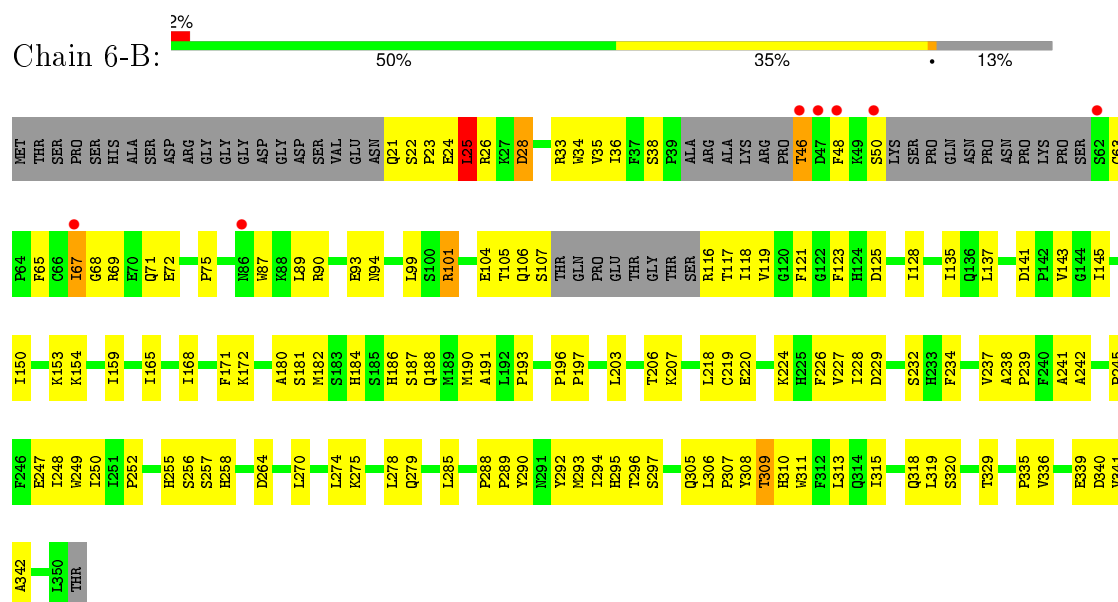




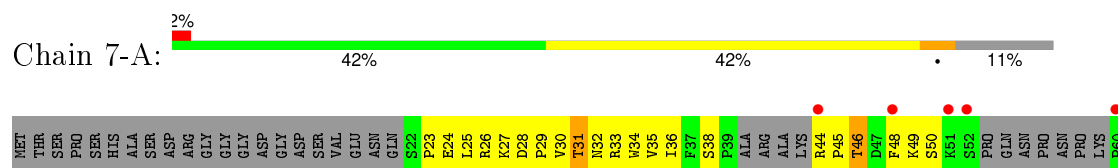
- Molecule 1: Probable galactose-1-phosphate uridyl transferase



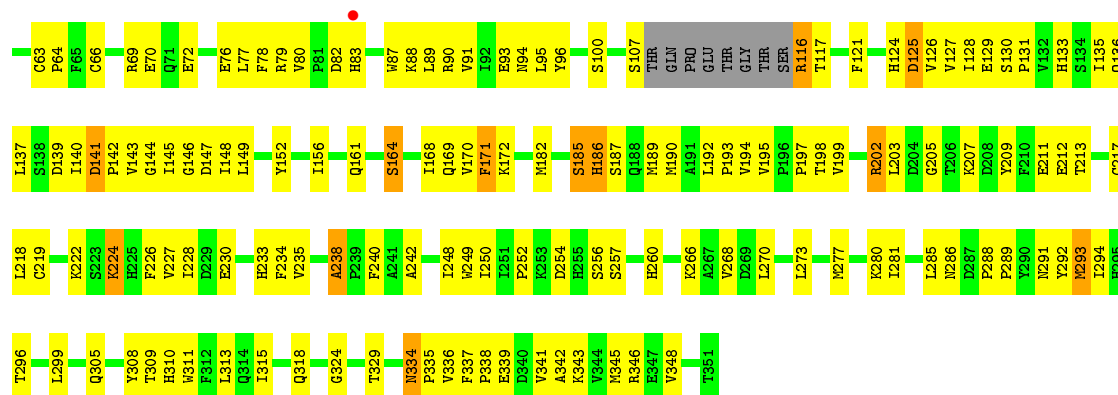
- Molecule 1: Probable galactose-1-phosphate uridyl transferase



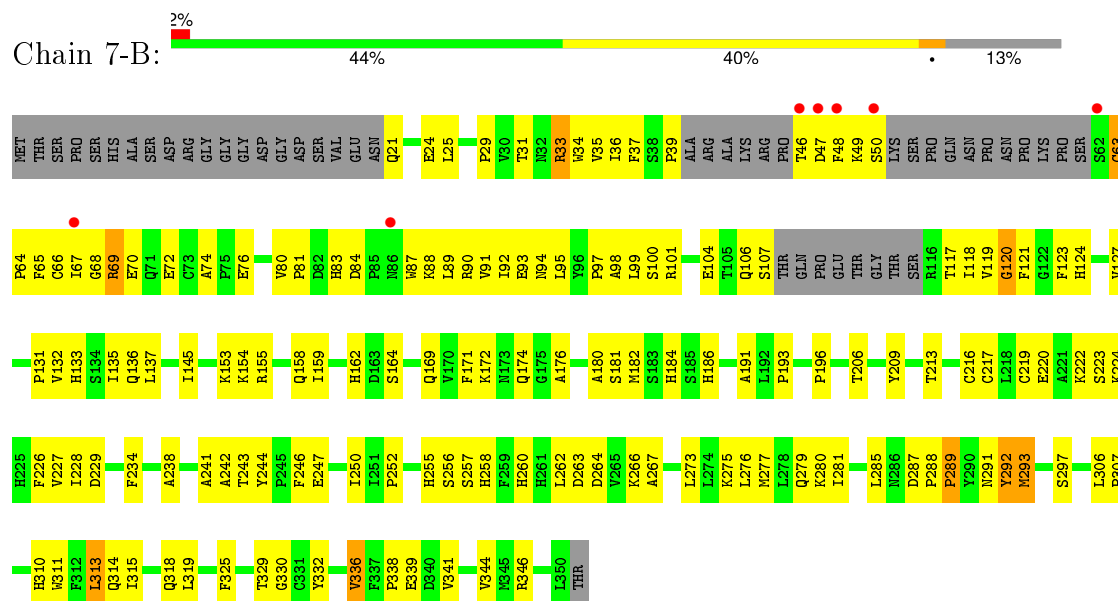
- Molecule 1: Probable galactose-1-phosphate uridyl transferase



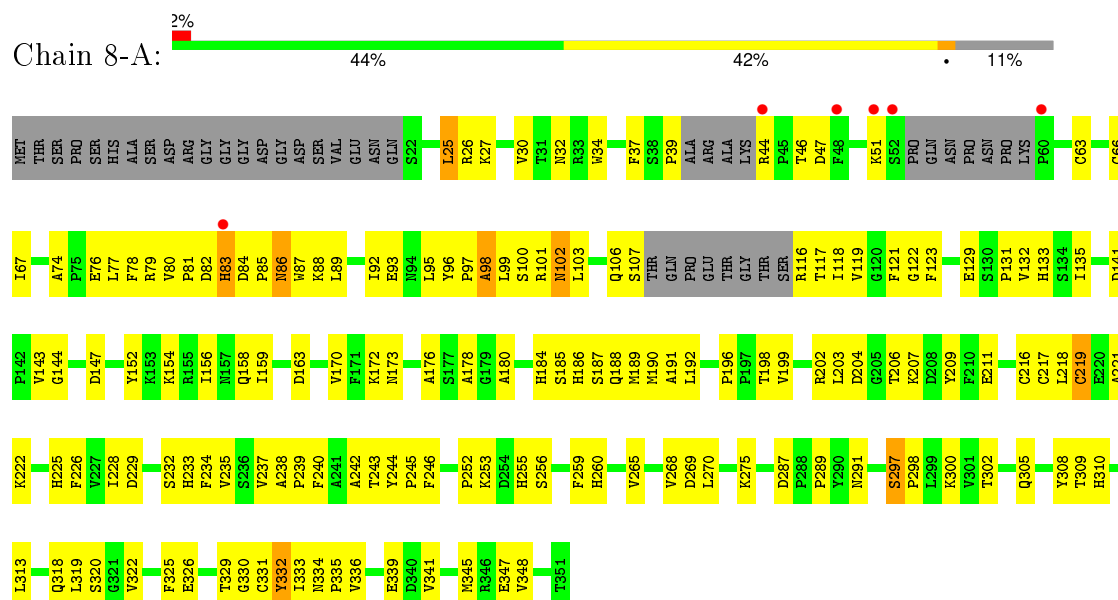




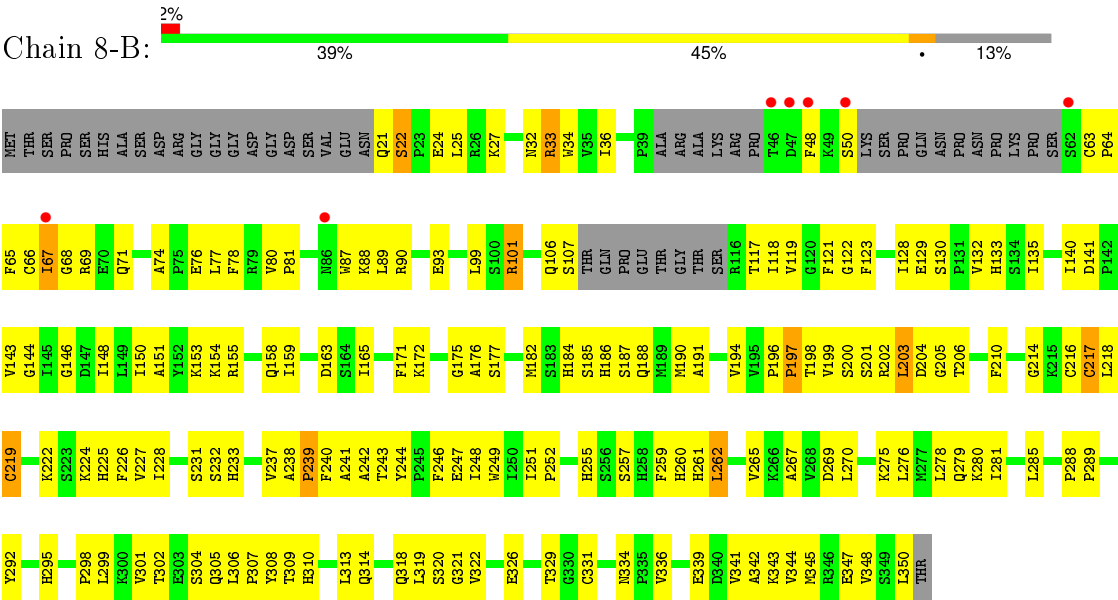
- Molecule 1: Probable galactose-1-phosphate uridyl transferase



- Molecule 1: Probable galactose-1-phosphate uridyl transferase



● Molecule 1: Probable galactose-1-phosphate uridyl transferase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	62.04Å 95.65Å 110.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	31.28 – 1.83 31.28 – 1.83	Depositor EDS
% Data completeness (in resolution range)	97.9 (31.28-1.83) 98.0 (31.28-1.83)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.87 (at 1.83Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.154 , 0.218 0.161 , 0.219	Depositor DCC
$R_{free}$ test set	2903 reflections (5.32%)	DCC
Wilson B-factor (Å <sup>2</sup> )	22.6	Xtriage
Anisotropy	0.147	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	(Not available) , (Not available)	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 57442 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	43592	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.16% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: AMP, ZN, EDO

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-A	0.74	0/2529	0.80	2/3434 (0.1%)
1	1-B	0.70	0/2482	0.82	5/3372 (0.1%)
1	2-A	0.75	0/2529	0.79	1/3434 (0.0%)
1	2-B	0.69	0/2482	0.77	2/3372 (0.1%)
1	3-A	0.73	0/2529	0.81	0/3434
1	3-B	0.68	0/2482	0.79	1/3372 (0.0%)
1	4-A	0.73	0/2529	0.79	1/3434 (0.0%)
1	4-B	0.71	0/2482	0.80	2/3372 (0.1%)
1	5-A	0.82	2/2529 (0.1%)	0.84	1/3434 (0.0%)
1	5-B	0.76	0/2482	0.85	4/3372 (0.1%)
1	6-A	0.82	1/2529 (0.0%)	0.88	1/3434 (0.0%)
1	6-B	0.73	0/2482	0.82	2/3372 (0.1%)
1	7-A	0.80	0/2529	0.83	1/3434 (0.0%)
1	7-B	0.76	0/2482	0.85	6/3372 (0.2%)
1	8-A	0.79	1/2529 (0.0%)	0.83	2/3434 (0.1%)
1	8-B	0.74	1/2482 (0.0%)	0.86	4/3372 (0.1%)
All	All	0.75	5/40088 (0.0%)	0.82	35/54448 (0.1%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	6-A	219	CYS	CB-SG	-9.82	1.65	1.82
1	5-A	216	CYS	CB-SG	8.00	1.95	1.82
1	8-A	219	CYS	CB-SG	-5.46	1.73	1.81
1	5-A	139	ASP	CB-CG	5.13	1.62	1.51
1	8-B	219	CYS	CB-SG	-5.08	1.73	1.81

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	7-B	33	ARG	NE-CZ-NH2	-9.58	115.51	120.30
1	8-B	33	ARG	NE-CZ-NH2	-9.17	115.72	120.30
1	6-A	219	CYS	CA-CB-SG	-8.61	98.51	114.00
1	1-B	33	ARG	NE-CZ-NH2	-8.42	116.09	120.30
1	4-B	33	ARG	NE-CZ-NH2	-8.22	116.19	120.30
1	5-B	33	ARG	NE-CZ-NH2	-8.05	116.28	120.30
1	7-B	33	ARG	NE-CZ-NH1	6.72	123.66	120.30
1	5-B	33	ARG	NE-CZ-NH1	6.41	123.51	120.30
1	6-B	25	LEU	CA-CB-CG	6.39	130.01	115.30
1	3-B	238	ALA	N-CA-C	-6.32	93.94	111.00
1	8-A	289	PRO	N-CA-C	-6.11	96.21	112.10
1	5-B	238	ALA	N-CA-C	-6.09	94.56	111.00
1	8-B	313	LEU	CA-CB-CG	6.07	129.26	115.30
1	1-B	236	SER	N-CA-C	-6.06	94.65	111.00
1	1-B	101	ARG	NE-CZ-NH1	-5.95	117.33	120.30
1	8-B	33	ARG	NE-CZ-NH1	5.89	123.24	120.30
1	2-A	298	PRO	N-CA-C	-5.78	97.08	112.10
1	1-A	238	ALA	N-CA-C	-5.74	95.51	111.00
1	7-B	238	ALA	N-CA-C	-5.62	95.83	111.00
1	2-B	238	ALA	N-CA-C	-5.55	96.03	111.00
1	5-B	101	ARG	NE-CZ-NH2	5.55	123.07	120.30
1	6-B	238	ALA	N-CA-C	-5.48	96.20	111.00
1	1-A	289	PRO	N-CA-C	-5.36	98.18	112.10
1	4-B	238	ALA	N-CA-C	-5.33	96.60	111.00
1	8-A	238	ALA	N-CA-C	-5.33	96.60	111.00
1	4-A	289	PRO	N-CA-C	-5.32	98.28	112.10
1	5-A	289	PRO	N-CA-C	-5.28	98.38	112.10
1	2-B	313	LEU	CA-CB-CG	5.27	127.42	115.30
1	8-B	239	PRO	N-CA-C	5.18	125.58	112.10
1	1-B	101	ARG	NE-CZ-NH2	5.17	122.89	120.30
1	7-B	313	LEU	CA-CB-CG	5.14	127.11	115.30
1	7-B	262	LEU	CA-CB-CG	5.13	127.11	115.30
1	7-B	289	PRO	N-CA-C	-5.11	98.80	112.10
1	7-A	238	ALA	N-CA-C	-5.08	97.30	111.00
1	1-B	33	ARG	NE-CZ-NH1	5.03	122.81	120.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1-A	2461	0	2421	162	0
1	1-B	2416	0	2369	191	0
1	2-A	2461	0	2420	164	0
1	2-B	2416	0	2369	178	0
1	3-A	2461	0	2419	190	0
1	3-B	2416	0	2370	185	0
1	4-A	2461	0	2421	191	0
1	4-B	2416	0	2369	141	0
1	5-A	2461	0	2421	194	0
1	5-B	2416	0	2369	176	0
1	6-A	2461	0	2420	233	0
1	6-B	2416	0	2370	152	0
1	7-A	2461	0	2420	190	0
1	7-B	2416	0	2370	161	0
1	8-A	2461	0	2421	149	0
1	8-B	2416	0	2370	195	0
2	1-A	2	0	0	0	0
2	1-B	2	0	0	0	0
2	2-A	2	0	0	0	0
2	2-B	2	0	0	0	0
2	3-A	2	0	0	0	0
2	3-B	2	0	0	0	0
2	4-A	2	0	0	0	0
2	4-B	2	0	0	0	0
2	5-A	2	0	0	1	0
2	5-B	2	0	0	0	0
2	6-A	2	0	0	0	0
2	6-B	2	0	0	0	0
2	7-A	2	0	0	0	0
2	7-B	2	0	0	0	0
2	8-A	2	0	0	0	0
2	8-B	2	0	0	0	0
3	1-A	22	0	12	7	0
3	1-B	22	0	12	6	0
3	2-A	22	0	12	7	0
3	2-B	22	0	12	5	0
3	3-A	22	0	12	4	0
3	3-B	22	0	12	6	0
3	4-A	22	0	12	5	0
3	4-B	22	0	12	5	0
3	5-A	22	0	11	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	5-B	22	0	11	3	0
3	6-A	22	0	11	6	0
3	6-B	22	0	11	7	0
3	7-A	22	0	11	4	0
3	7-B	22	0	12	5	0
3	8-A	22	0	11	5	0
3	8-B	22	0	11	4	0
4	1-A	12	0	18	0	0
4	1-B	12	0	18	1	0
4	2-A	12	0	18	1	0
4	2-B	12	0	18	0	0
4	3-A	12	0	18	3	0
4	3-B	12	0	18	5	0
4	4-A	12	0	18	3	0
4	4-B	12	0	18	2	0
4	5-A	12	0	18	2	0
4	5-B	12	0	18	5	0
4	6-A	12	0	18	2	0
4	6-B	12	0	18	3	0
4	7-A	12	0	18	3	0
4	7-B	12	0	18	4	0
4	8-A	12	0	18	5	0
4	8-B	12	0	18	4	0
5	1-A	273	0	0	17	0
5	1-B	227	0	0	24	0
5	2-A	274	0	0	22	0
5	2-B	226	0	0	20	0
5	3-A	270	0	0	25	0
5	3-B	230	0	0	22	0
5	4-A	272	0	0	28	0
5	4-B	228	0	0	10	0
5	5-A	270	0	0	26	0
5	5-B	230	0	0	16	0
5	6-A	270	0	0	35	0
5	6-B	230	0	0	28	0
5	7-A	270	0	0	28	0
5	7-B	230	0	0	19	0
5	8-A	271	0	0	19	0
5	8-B	229	0	0	33	0
All	All	43592	0	38792	2702	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 34.

All (2702) 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:A:186:HIS:NE2	3:A:601:AMP:P	2.11	1.24
1:B:186:HIS:NE2	3:B:602:AMP:P	2.11	1.23
1:A:116:ARG:HB2	1:A:116:ARG:NH2	1.58	1.18
1:A:239:PRO:HB2	1:A:242:ALA:HB2	1.26	1.12
1:A:119:VAL:HG13	5:A:700:HOH:O	1.51	1.11
1:B:71:GLN:HB2	5:B:714:HOH:O	1.52	1.10
1:B:155:ARG:HA	1:B:158:GLN:OE1	1.49	1.10
1:A:76:GLU:HA	1:A:92:ILE:HG22	1.30	1.09
1:B:90:ARG:NH2	5:B:796:HOH:O	1.87	1.08
1:B:33:ARG:HG3	1:B:33:ARG:HH11	1.03	1.07
1:B:71:GLN:HB2	5:B:715:HOH:O	1.56	1.05
1:B:172:LYS:HB3	1:B:292:TYR:HB3	1.32	1.04
1:B:219:CYS:SG	1:B:220:GLU:HG3	1.97	1.03
1:B:65:PHE:O	5:B:796:HOH:O	1.78	1.01
1:B:186:HIS:CE1	3:B:602:AMP:P	2.53	1.01
1:A:256:SER:HB3	5:A:877:HOH:O	1.56	1.01
1:B:252:PRO:HG2	1:B:310:HIS:HE2	1.20	1.01
1:A:186:HIS:NE2	3:A:601:AMP:P	2.32	1.01
1:B:119:VAL:HG13	5:B:781:HOH:O	1.61	1.01
1:A:186:HIS:CE1	3:A:601:AMP:P	2.54	1.01
1:B:90:ARG:NH2	5:B:794:HOH:O	1.94	1.00
1:B:33:ARG:HD2	5:B:705:HOH:O	1.61	1.00
1:A:99:LEU:HD21	1:B:36:ILE:HD13	1.41	1.00
1:B:101:ARG:HD2	5:B:714:HOH:O	1.60	1.00
1:A:169:GLN:NE2	1:B:329:THR:HG23	1.75	0.99
1:A:337:PHE:HB3	1:A:339:GLU:OE1	1.62	0.99
1:A:219:CYS:HA	5:A:653:HOH:O	1.62	0.98
1:B:346:ARG:HB2	1:B:346:ARG:NH1	1.79	0.98
1:B:49:LYS:HD3	1:B:286:ASN:HD21	1.25	0.97
1:B:30:VAL:HG13	1:B:202:ARG:HD3	1.43	0.97
1:A:219:CYS:HB3	1:A:310:HIS:CE1	1.98	0.97
1:B:224:LYS:HE2	1:B:224:LYS:HA	1.47	0.96
1:B:250:ILE:HD12	1:B:313:LEU:HD22	1.43	0.96
1:A:127:VAL:HB	1:A:187:SER:HB2	1.44	0.95
1:B:292:TYR:N	1:B:293:MET:HE3	1.81	0.95
1:B:186:HIS:NE2	3:B:602:AMP:P	2.40	0.94
1:B:346:ARG:HH11	1:B:346:ARG:CB	1.81	0.94
1:A:281:ILE:HG23	1:A:285:LEU:HD12	1.50	0.94
1:B:186:HIS:NE2	3:B:602:AMP:P	2.41	0.94
1:B:250:ILE:HD11	1:B:277:MET:HG3	1.50	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:186:HIS:NE2	3:A:601:AMP:P	2.41	0.93
1:A:219:CYS:HB3	1:A:310:HIS:HE1	1.30	0.93
1:B:119:VAL:HG13	5:B:785:HOH:O	1.67	0.93
1:B:346:ARG:HH11	1:B:346:ARG:HB2	1.34	0.93
1:A:256:SER:HB3	5:A:876:HOH:O	1.68	0.93
1:B:217:CYS:SG	5:B:660:HOH:O	2.26	0.92
1:A:196:PRO:HB2	1:B:329:THR:HB	1.50	0.92
1:B:217:CYS:HB2	1:B:224:LYS:HE2	1.51	0.92
1:B:34:TRP:HB2	5:B:784:HOH:O	1.67	0.92
1:B:292:TYR:HE2	1:B:294:ILE:HG13	1.34	0.92
1:B:281:ILE:HG23	1:B:285:LEU:HD12	1.51	0.91
1:B:67:ILE:HD13	1:B:87:TRP:NE1	1.86	0.91
1:A:116:ARG:HB2	1:A:116:ARG:HH21	1.28	0.91
1:B:46:THR:HB	1:B:344:VAL:HG21	1.51	0.91
1:A:116:ARG:HD3	5:A:820:HOH:O	1.72	0.90
1:A:147:ASP:OD1	5:A:715:HOH:O	1.88	0.90
1:B:127:VAL:O	1:B:186:HIS:HA	1.72	0.90
1:B:129:GLU:OE2	1:B:185:SER:HB2	1.70	0.90
1:B:119:VAL:HG13	5:B:788:HOH:O	1.70	0.90
1:A:331:CYS:HB2	1:B:197:PRO:HD2	1.51	0.90
1:A:143:VAL:HG23	5:A:673:HOH:O	1.72	0.90
1:B:48:PHE:HB2	1:B:336:VAL:HG21	1.54	0.90
1:B:107:SER:HB3	1:B:119:VAL:HG22	1.53	0.89
1:B:65:PHE:O	5:B:796:HOH:O	1.89	0.89
1:B:172:LYS:HE3	1:B:174:GLN:HB2	1.55	0.89
1:A:172:LYS:O	1:A:291:ASN:HB3	1.73	0.89
1:A:251:ILE:HG22	1:A:252:PRO:HD2	1.54	0.89
1:B:252:PRO:HG2	1:B:310:HIS:NE2	1.87	0.89
1:A:216:CYS:HG	2:A:604:ZN:ZN	0.84	0.89
1:A:256:SER:H	1:A:310:HIS:CD2	1.90	0.89
1:A:224:LYS:HE3	5:A:880:HOH:O	1.73	0.88
1:B:119:VAL:HG13	5:B:785:HOH:O	1.72	0.88
1:B:25:LEU:HD22	1:B:36:ILE:HG12	1.55	0.88
1:A:143:VAL:HG23	5:A:674:HOH:O	1.72	0.88
1:A:119:VAL:HG13	5:A:701:HOH:O	1.71	0.88
1:A:186:HIS:NE2	3:A:601:AMP:P	2.47	0.88
1:A:213:THR:HB	1:A:215:LYS:HE3	1.54	0.88
1:A:186:HIS:NE2	3:A:601:AMP:O1P	2.07	0.87
1:B:257:SER:O	1:B:311:TRP:HB3	1.75	0.87
1:B:322:VAL:HG22	5:B:674:HOH:O	1.74	0.87
1:A:170:VAL:HG22	1:A:189:MET:HE2	1.56	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:281:ILE:HG23	1:A:285:LEU:HD12	1.57	0.87
1:A:213:THR:HB	1:A:215:LYS:HE3	1.56	0.87
1:A:88:LYS:HD2	5:A:714:HOH:O	1.72	0.87
1:B:256:SER:O	1:B:310:HIS:HA	1.75	0.87
1:A:256:SER:CB	5:A:874:HOH:O	2.23	0.87
1:B:292:TYR:CE2	1:B:294:ILE:HG13	2.09	0.86
1:B:33:ARG:HG3	1:B:33:ARG:NH1	1.81	0.86
1:A:116:ARG:HD3	5:A:822:HOH:O	1.74	0.86
1:A:116:ARG:HH21	1:A:117:THR:H	1.23	0.86
1:A:334:ASN:ND2	1:A:336:VAL:H	1.72	0.86
1:A:222:LYS:HG2	1:A:235:VAL:HG21	1.57	0.86
1:A:343:LYS:HA	1:A:346:ARG:HD2	1.58	0.86
1:B:66:CYS:SG	1:B:133:HIS:HB2	2.15	0.86
1:B:33:ARG:CG	1:B:33:ARG:HH11	1.86	0.86
1:B:171:PHE:HE1	1:B:173:ASN:HD21	1.25	0.85
1:B:135:ILE:O	5:B:694:HOH:O	1.94	0.85
1:A:117:THR:HG21	1:B:24:GLU:OE1	1.74	0.85
1:B:228:ILE:HG12	1:B:342:ALA:HA	1.58	0.85
1:A:169:GLN:NE2	1:A:293:MET:HB3	1.92	0.84
1:B:186:HIS:CE1	3:B:602:AMP:P	2.70	0.84
1:A:38:SER:O	1:A:335:PRO:HA	1.77	0.84
1:A:51:LYS:HG2	5:A:771:HOH:O	1.77	0.84
1:B:33:ARG:NH2	1:B:243:THR:OG1	2.10	0.84
1:B:93:GLU:HG2	1:B:101:ARG:HH21	1.43	0.84
1:B:248:ILE:HD11	1:B:345:MET:HE2	1.58	0.84
1:A:235:VAL:O	1:A:237:VAL:HG13	1.77	0.84
1:A:64:PRO:O	5:A:660:HOH:O	1.94	0.84
1:A:258:HIS:HB3	1:A:260:HIS:CE1	2.13	0.84
1:B:218:LEU:HD12	1:B:310:HIS:HB3	1.60	0.83
1:B:235:VAL:O	1:B:237:VAL:HG13	1.78	0.83
1:A:169:GLN:HE22	1:B:329:THR:N	1.75	0.83
1:A:324:GLY:H	1:B:291:ASN:ND2	1.75	0.83
1:B:181:SER:N	3:B:602:AMP:O2P	2.12	0.83
1:B:94:ASN:O	1:B:97:PRO:HD3	1.77	0.83
1:A:147:ASP:OD1	5:A:714:HOH:O	1.96	0.83
1:B:33:ARG:HB3	5:B:711:HOH:O	1.76	0.83
1:A:49:LYS:HD2	1:A:286:ASN:OD1	1.79	0.83
1:B:181:SER:N	3:B:602:AMP:O2P	2.11	0.83
1:A:213:THR:HB	1:A:215:LYS:CE	2.09	0.83
1:B:182:MET:HB2	1:B:186:HIS:CE1	2.12	0.83
1:B:240:PHE:HA	1:B:338:PRO:HG3	1.59	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:88:LYS:HD2	5:A:714:HOH:O	1.79	0.82
1:A:225:HIS:ND1	1:A:240:PHE:N	2.26	0.82
1:A:161:GLN:HG3	5:A:787:HOH:O	1.78	0.82
1:A:280:LYS:HG2	1:A:350:LEU:HD11	1.60	0.82
1:A:171:PHE:CB	1:A:293:MET:HG3	2.10	0.82
1:A:99:LEU:HD21	1:B:25:LEU:HD21	1.61	0.82
1:A:125:ASP:OD2	1:A:189:MET:HB2	1.80	0.82
1:A:28:ASP:HB2	1:A:241:ALA:HB3	1.60	0.82
1:B:49:LYS:HB3	1:B:286:ASN:HD22	1.45	0.82
1:B:242:ALA:HB3	4:B:610:EDO:H21	1.61	0.81
1:A:216:CYS:HB3	1:A:219:CYS:HB3	1.62	0.81
1:A:333:ILE:HG22	1:A:335:PRO:HD3	1.61	0.81
1:A:174:GLN:C	1:A:174:GLN:HE21	1.83	0.81
1:A:249:TRP:NE1	1:A:314:GLN:HG3	1.95	0.81
1:A:162:HIS:C	1:A:164:SER:H	1.84	0.81
1:A:228:ILE:HG13	1:A:237:VAL:HA	1.63	0.81
1:B:165:ILE:HG22	1:B:299:LEU:HD11	1.61	0.81
1:B:21:GLN:HG2	5:B:767:HOH:O	1.81	0.81
1:A:90:ARG:HB2	1:A:128:ILE:HD12	1.61	0.80
1:A:170:VAL:HG22	1:A:189:MET:HG2	1.61	0.80
1:B:93:GLU:HG2	1:B:101:ARG:NH2	1.96	0.80
1:A:194:VAL:HB	5:A:744:HOH:O	1.80	0.80
1:A:196:PRO:CB	1:B:329:THR:HB	2.11	0.80
1:A:248:ILE:HD12	1:A:281:ILE:HD11	1.63	0.80
1:B:318:GLN:HG3	4:B:612:EDO:O2	1.82	0.80
1:A:170:VAL:HB	1:A:294:ILE:HD12	1.64	0.80
1:A:61:SER:O	5:A:754:HOH:O	2.00	0.80
1:B:46:THR:HG23	1:B:47:ASP:H	1.46	0.80
1:A:121:PHE:HE2	1:A:164:SER:HG	1.30	0.80
1:B:31:THR:HG22	4:B:611:EDO:H11	1.63	0.80
1:A:227:VAL:HA	1:A:237:VAL:HG12	1.64	0.79
1:A:39:PRO:HA	1:A:335:PRO:O	1.82	0.79
1:A:302:THR:O	1:A:306:LEU:HG	1.81	0.79
1:B:25:LEU:HD11	1:B:36:ILE:HG12	1.62	0.79
1:A:45:PRO:HA	1:A:48:PHE:CE2	2.18	0.79
1:B:245:PRO:HG2	5:B:632:HOH:O	1.81	0.79
1:A:249:TRP:HE1	1:A:314:GLN:HG3	1.47	0.79
1:A:302:THR:OG1	1:A:305:GLN:HG3	1.81	0.79
1:B:234:PHE:HB2	1:B:273:LEU:HD22	1.65	0.79
1:A:217:CYS:HA	1:A:220:GLU:HG2	1.63	0.79
1:A:273:LEU:O	1:A:277:MET:HG2	1.81	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:147:ASP:OD1	5:A:713:HOH:O	2.00	0.79
1:B:172:LYS:O	1:B:291:ASN:HA	1.82	0.79
1:B:106:GLN:O	1:B:107:SER:HB2	1.81	0.79
1:A:257:SER:O	1:A:297:SER:HB2	1.83	0.79
1:A:119:VAL:HG13	5:A:702:HOH:O	1.83	0.79
1:B:49:LYS:HG2	1:B:285:LEU:HA	1.64	0.78
1:A:25:LEU:HD13	1:B:118:ILE:HD11	1.63	0.78
1:A:62:SER:HA	1:A:66:CYS:SG	2.24	0.78
1:A:127:VAL:HB	1:A:187:SER:CB	2.13	0.78
1:B:91:VAL:HG22	1:B:127:VAL:HG22	1.65	0.78
1:B:292:TYR:H	1:B:293:MET:HE3	1.47	0.78
1:B:344:VAL:HG13	5:B:676:HOH:O	1.83	0.78
1:A:247:GLU:C	1:A:248:ILE:HD12	2.04	0.78
1:A:285:LEU:O	1:A:288:PRO:HD3	1.84	0.78
1:A:50:SER:HB2	1:A:288:PRO:HB3	1.66	0.78
1:A:25:LEU:HB2	1:B:118:ILE:CG1	2.14	0.78
1:B:50:SER:CB	1:B:288:PRO:HB3	2.13	0.78
1:B:30:VAL:HG21	1:B:218:LEU:HD21	1.67	0.77
1:A:35:VAL:HA	1:A:331:CYS:SG	2.24	0.77
1:A:116:ARG:HB2	1:A:116:ARG:CZ	2.12	0.77
1:B:66:CYS:SG	1:B:133:HIS:HB2	2.25	0.77
1:B:341:VAL:HG21	4:B:610:EDO:O1	1.83	0.77
1:A:325:PHE:CE1	1:B:190:MET:HG2	2.20	0.77
1:B:70:GLU:HG3	1:B:90:ARG:CZ	2.13	0.77
1:A:252:PRO:HG3	1:A:311:TRP:NE1	2.00	0.77
1:A:300:LYS:HG2	5:A:620:HOH:O	1.85	0.77
1:A:123:PHE:HB2	1:A:191:ALA:HB3	1.67	0.77
1:B:281:ILE:HG23	1:B:285:LEU:HD12	1.64	0.77
1:B:25:LEU:HD21	1:B:36:ILE:HD13	1.65	0.77
1:A:306:LEU:HB2	1:A:307:PRO:HD3	1.65	0.77
1:B:132:VAL:HB	1:B:135:ILE:HD12	1.65	0.77
1:B:21:GLN:HG2	1:B:22:SER:H	1.49	0.77
1:A:116:ARG:HD2	5:A:822:HOH:O	1.82	0.76
1:B:65:PHE:O	5:B:797:HOH:O	2.03	0.76
1:A:302:THR:HG21	5:A:868:HOH:O	1.86	0.76
1:B:101:ARG:HD2	5:B:720:HOH:O	1.86	0.76
1:A:129:GLU:HG3	1:A:186:HIS:HA	1.67	0.76
1:A:279:GLN:HG2	1:A:350:LEU:HD13	1.68	0.76
1:A:181:SER:N	3:A:601:AMP:O2P	2.18	0.76
1:B:182:MET:SD	3:B:602:AMP:H5'1	2.25	0.76
1:A:252:PRO:HG2	1:A:310:HIS:CE1	2.20	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:141:ASP:OD1	5:A:724:HOH:O	2.02	0.76
1:A:167:TYR:HE2	1:A:296:THR:O	1.68	0.76
1:B:153:LYS:HD3	5:B:695:HOH:O	1.86	0.76
1:A:346:ARG:HD3	5:A:881:HOH:O	1.86	0.76
1:B:287:ASP:HA	5:B:628:HOH:O	1.85	0.75
1:A:249:TRP:HA	1:A:313:LEU:O	1.86	0.75
1:A:277:MET:HA	1:A:277:MET:CE	2.16	0.75
1:B:177:SER:CB	1:B:318:GLN:HE22	1.99	0.75
1:B:127:VAL:HB	1:B:187:SER:HB2	1.67	0.75
1:A:197:PRO:HG2	1:B:330:GLY:O	1.86	0.75
1:A:99:LEU:HD12	1:A:122:GLY:HA3	1.67	0.75
1:B:25:LEU:HD11	1:B:36:ILE:HG12	1.65	0.75
1:B:69:ARG:O	1:B:72:GLU:HB3	1.86	0.75
1:B:143:VAL:HA	1:B:268:VAL:HG13	1.68	0.75
1:B:276:LEU:O	1:B:279:GLN:N	2.20	0.75
1:B:67:ILE:HD12	1:B:68:GLY:N	2.01	0.75
1:A:342:ALA:O	1:A:346:ARG:HG3	1.87	0.75
1:B:213:THR:OG1	1:B:215:LYS:HG2	1.86	0.75
1:B:273:LEU:HD12	1:B:277:MET:HE3	1.69	0.75
1:A:66:CYS:SG	1:A:133:HIS:HB2	2.27	0.75
1:B:184:HIS:O	1:B:186:HIS:CD2	2.39	0.75
1:A:250:ILE:HB	1:A:313:LEU:HB3	1.67	0.75
1:A:329:THR:HB	1:B:196:PRO:CB	2.17	0.74
1:B:219:CYS:SG	5:B:830:HOH:O	2.44	0.74
1:B:21:GLN:HG2	1:B:22:SER:H	1.51	0.74
1:B:129:GLU:HB2	1:B:185:SER:OG	1.87	0.74
1:B:119:VAL:HG23	5:B:687:HOH:O	1.86	0.74
1:B:106:GLN:O	1:B:107:SER:HB2	1.87	0.74
1:A:172:LYS:O	1:A:291:ASN:HA	1.88	0.74
1:B:250:ILE:HB	1:B:313:LEU:HB3	1.67	0.74
1:A:127:VAL:N	1:A:187:SER:O	2.14	0.74
1:A:256:SER:OG	5:A:874:HOH:O	2.05	0.74
1:A:106:GLN:HB2	1:A:119:VAL:HG11	1.70	0.74
1:B:176:ALA:HA	1:B:180:ALA:O	1.88	0.74
1:A:99:LEU:HD13	1:A:121:PHE:O	1.87	0.74
1:B:25:LEU:HD13	1:B:36:ILE:HA	1.68	0.74
1:B:106:GLN:HB3	1:B:119:VAL:HG11	1.70	0.74
1:A:322:VAL:HB	1:A:326:GLU:HB2	1.69	0.74
1:A:186:HIS:NE2	3:A:601:AMP:O1P	2.20	0.74
1:A:27:LYS:HE2	1:A:32:ASN:C	2.08	0.74
1:A:129:GLU:OE2	1:A:185:SER:C	2.26	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:202:ARG:CZ	1:B:295:HIS:HB3	2.17	0.74
1:A:107:SER:HA	1:A:121:PHE:CE2	2.23	0.74
1:A:282:ALA:HB1	1:A:287:ASP:OD1	1.88	0.74
1:A:322:VAL:HB	1:A:326:GLU:OE2	1.88	0.73
1:A:331:CYS:HB2	1:B:197:PRO:CD	2.18	0.73
1:B:216:CYS:HB3	1:B:219:CYS:HB3	1.70	0.73
1:A:218:LEU:HD22	1:A:251:ILE:HD13	1.70	0.73
1:B:25:LEU:CD2	1:B:36:ILE:HG12	2.18	0.73
1:A:147:ASP:OD1	5:A:714:HOH:O	2.06	0.73
1:A:222:LYS:HD2	5:A:873:HOH:O	1.87	0.73
1:A:99:LEU:HD13	1:A:121:PHE:O	1.87	0.73
1:B:172:LYS:O	1:B:291:ASN:HA	1.89	0.73
1:A:67:ILE:HD12	1:A:131:PRO:HB3	1.70	0.73
1:A:329:THR:O	1:B:197:PRO:HB2	1.89	0.73
1:B:76:GLU:HA	1:B:92:ILE:HG22	1.68	0.73
1:B:246:PHE:CD2	1:B:285:LEU:HD11	2.22	0.73
1:A:329:THR:HG22	1:B:196:PRO:HG3	1.68	0.73
1:B:186:HIS:ND1	3:B:602:AMP:P	2.62	0.73
1:B:33:ARG:HD3	5:B:712:HOH:O	1.89	0.73
1:A:127:VAL:CB	1:A:187:SER:HB2	2.19	0.73
1:A:30:VAL:HG13	1:A:202:ARG:HG3	1.71	0.73
1:A:80:VAL:HB	1:A:89:LEU:HG	1.69	0.73
1:B:90:ARG:HD3	5:B:796:HOH:O	1.89	0.73
1:A:249:TRP:HB3	1:A:251:ILE:HD11	1.70	0.73
1:B:129:GLU:OE2	1:B:137:LEU:HB2	1.87	0.73
1:A:66:CYS:SG	1:A:133:HIS:HB2	2.28	0.73
1:B:247:GLU:OE1	1:B:249:TRP:NE1	2.21	0.73
1:B:213:THR:HB	1:B:215:LYS:HE2	1.71	0.72
1:B:188:GLN:NE2	3:B:602:AMP:O1P	2.21	0.72
1:B:66:CYS:SG	1:B:133:HIS:HB2	2.29	0.72
1:A:257:SER:HA	1:A:309:THR:O	1.89	0.72
1:A:49:LYS:HD2	1:A:286:ASN:ND2	2.04	0.72
1:B:245:PRO:HA	4:B:610:EDO:O2	1.90	0.72
1:B:186:HIS:HE1	3:B:602:AMP:P	2.10	0.72
1:A:116:ARG:NH2	1:A:117:THR:H	1.88	0.72
1:A:254:ASP:OD2	5:A:861:HOH:O	2.07	0.72
1:A:346:ARG:HD3	5:A:878:HOH:O	1.88	0.72
1:B:67:ILE:HD13	1:B:87:TRP:HE1	1.54	0.72
1:B:173:ASN:O	1:B:180:ALA:HB2	1.89	0.72
1:B:206:THR:O	5:B:677:HOH:O	2.07	0.72
1:B:32:ASN:HB3	1:B:201:SER:HB3	1.70	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:21:GLN:OE1	5:B:777:HOH:O	2.07	0.72
1:A:66:CYS:SG	1:A:133:HIS:HB2	2.28	0.72
1:B:174:GLN:OE1	5:B:634:HOH:O	2.08	0.72
1:B:49:LYS:HD3	1:B:286:ASN:ND2	2.02	0.72
1:B:21:GLN:NE2	5:B:766:HOH:O	2.23	0.72
1:B:106:GLN:HG3	5:B:803:HOH:O	1.90	0.72
1:A:167:TYR:CZ	1:A:199:VAL:HG21	2.25	0.72
1:B:136:GLN:HG2	5:B:722:HOH:O	1.88	0.71
1:B:100:SER:HB3	1:B:103:LEU:HD12	1.72	0.71
1:A:301:VAL:HA	1:A:305:GLN:OE1	1.90	0.71
1:B:46:THR:HG22	1:B:344:VAL:HG21	1.70	0.71
1:B:66:CYS:O	5:B:715:HOH:O	2.08	0.71
1:B:275:LYS:HE3	1:B:279:GLN:OE1	1.91	0.71
1:A:146:GLY:O	1:A:150:ILE:HG12	1.90	0.71
1:B:25:LEU:HD13	1:B:36:ILE:HA	1.70	0.71
1:B:154:LYS:O	1:B:158:GLN:HG3	1.91	0.71
1:A:117:THR:OG1	1:B:24:GLU:HG2	1.91	0.71
1:A:284:GLN:OE1	5:A:708:HOH:O	2.08	0.71
1:B:175:GLY:HA3	1:B:289:PRO:HB3	1.73	0.71
1:B:33:ARG:HH22	1:B:243:THR:HG1	1.36	0.71
1:B:186:HIS:CE1	3:B:602:AMP:P	2.84	0.71
1:A:45:PRO:HA	1:A:48:PHE:CD2	2.25	0.71
1:B:76:GLU:OE1	5:B:717:HOH:O	2.09	0.71
1:A:207:LYS:HE2	1:A:211:GLU:OE1	1.89	0.71
1:A:227:VAL:HG23	5:A:681:HOH:O	1.90	0.71
1:A:100:SER:HB3	1:A:103:LEU:HD12	1.71	0.71
1:A:171:PHE:HB3	1:A:293:MET:HG3	1.71	0.71
1:B:36:ILE:HG22	1:B:37:PHE:N	2.04	0.71
1:B:193:PRO:HG2	1:B:194:VAL:HG13	1.73	0.71
1:B:181:SER:O	1:B:182:MET:HG3	1.91	0.71
1:A:299:LEU:C	1:A:300:LYS:HD3	2.12	0.70
1:B:21:GLN:O	1:B:22:SER:HB2	1.91	0.70
1:B:69:ARG:O	1:B:72:GLU:HB3	1.91	0.70
1:B:262:LEU:HD12	1:B:266:LYS:HB2	1.73	0.70
1:B:202:ARG:NH2	1:B:295:HIS:HB3	2.05	0.70
1:B:90:ARG:NH2	5:B:797:HOH:O	2.21	0.70
1:A:223:SER:HB3	5:A:801:HOH:O	1.91	0.70
1:B:239:PRO:HG3	1:B:249:TRP:CG	2.26	0.70
1:B:76:GLU:OE1	5:B:717:HOH:O	2.10	0.70
1:A:256:SER:N	1:A:310:HIS:CD2	2.59	0.70
1:B:331:CYS:SG	1:B:332:TYR:N	2.63	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:143:VAL:HG23	5:A:673:HOH:O	1.91	0.70
1:A:51:LYS:HE2	1:A:320:SER:HA	1.74	0.70
1:B:106:GLN:O	1:B:107:SER:HB2	1.91	0.70
1:B:135:ILE:O	5:B:694:HOH:O	2.08	0.70
1:B:175:GLY:HA3	1:B:289:PRO:HB3	1.73	0.70
1:A:167:TYR:CE2	1:A:199:VAL:HG21	2.26	0.70
1:B:69:ARG:O	1:B:72:GLU:HB3	1.91	0.70
1:B:76:GLU:OE1	5:B:711:HOH:O	2.10	0.70
1:B:165:ILE:CG2	1:B:299:LEU:HD11	2.21	0.70
1:A:198:THR:OG1	1:B:329:THR:HA	1.92	0.70
1:A:265:VAL:HG23	5:A:805:HOH:O	1.92	0.70
1:A:93:GLU:OE1	5:A:663:HOH:O	2.08	0.70
1:A:156:ILE:HG13	1:A:189:MET:CE	2.21	0.70
1:A:234:PHE:O	1:A:253:LYS:HE2	1.91	0.70
1:A:133:HIS:HE1	5:A:630:HOH:O	1.74	0.70
1:A:229:ASP:HB2	1:A:277:MET:HE1	1.74	0.70
1:A:334:ASN:HD22	1:A:335:PRO:N	1.89	0.69
1:A:351:THR:OXT	5:A:869:HOH:O	2.10	0.69
1:B:186:HIS:NE2	3:B:602:AMP:O1P	2.23	0.69
1:A:62:SER:OG	5:A:756:HOH:O	2.09	0.69
1:B:67:ILE:HB	1:B:131:PRO:HB2	1.72	0.69
1:A:153:LYS:HE3	5:A:706:HOH:O	1.91	0.69
1:A:228:ILE:HB	1:A:236:SER:OG	1.92	0.69
1:B:50:SER:HB3	1:B:285:LEU:O	1.91	0.69
1:B:285:LEU:HD22	1:B:319:LEU:HD21	1.73	0.69
1:A:69:ARG:HA	5:A:817:HOH:O	1.92	0.69
1:B:76:GLU:HA	1:B:92:ILE:HG22	1.73	0.69
1:A:228:ILE:HG12	1:A:342:ALA:HA	1.74	0.69
1:A:279:GLN:OE1	5:A:669:HOH:O	2.11	0.69
1:A:50:SER:HB2	1:A:288:PRO:HB3	1.74	0.69
1:B:186:HIS:CE1	3:B:602:AMP:P	2.86	0.69
1:A:236:SER:N	1:A:273:LEU:HD21	2.07	0.69
1:A:65:PHE:HE2	1:A:186:HIS:HD1	1.38	0.69
1:A:224:LYS:HB3	1:B:116:ARG:HH12	1.58	0.69
1:A:204:ASP:OD2	5:A:794:HOH:O	2.09	0.69
1:A:255:HIS:HA	1:A:310:HIS:CE1	2.27	0.69
1:A:163:ASP:OD2	5:A:732:HOH:O	2.09	0.69
1:B:186:HIS:NE2	3:B:602:AMP:O1P	2.24	0.69
1:A:301:VAL:HG22	1:A:305:GLN:HB2	1.74	0.69
1:A:219:CYS:CB	1:A:310:HIS:HE1	2.06	0.69
1:A:246:PHE:CD2	1:A:341:VAL:HG13	2.27	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:290:TYR:OH	5:A:627:HOH:O	2.11	0.69
1:A:30:VAL:HG21	1:A:218:LEU:HD21	1.74	0.69
1:A:251:ILE:HD12	1:A:251:ILE:N	2.08	0.69
1:B:207:LYS:HB2	1:B:308:TYR:CZ	2.27	0.69
1:A:256:SER:H	1:A:310:HIS:HD2	1.37	0.69
1:B:280:LYS:HG2	1:B:350:LEU:HD11	1.75	0.69
1:B:46:THR:HB	1:B:344:VAL:CG2	2.22	0.68
1:A:250:ILE:HD12	1:A:313:LEU:HD22	1.75	0.68
1:B:70:GLU:CD	1:B:70:GLU:H	1.95	0.68
1:A:305:GLN:HA	1:A:308:TYR:CZ	2.27	0.68
1:A:215:LYS:HD2	1:A:220:GLU:OE2	1.92	0.68
1:A:65:PHE:O	1:A:87:TRP:HH2	1.75	0.68
1:A:126:VAL:HG12	1:A:128:ILE:HG13	1.75	0.68
1:B:76:GLU:HB2	1:B:90:ARG:HH11	1.58	0.68
1:A:216:CYS:SG	1:A:255:HIS:ND1	2.65	0.68
1:A:224:LYS:HD2	5:A:878:HOH:O	1.93	0.68
1:A:171:PHE:HA	1:A:292:TYR:O	1.93	0.68
1:B:50:SER:HB3	1:B:286:ASN:HB3	1.75	0.68
1:A:329:THR:HB	1:B:196:PRO:HB3	1.74	0.68
1:B:25:LEU:HD13	1:B:36:ILE:HG12	1.75	0.68
1:A:121:PHE:CZ	1:A:164:SER:HB3	2.29	0.68
1:B:46:THR:HB	1:B:344:VAL:HG22	1.76	0.68
1:A:329:THR:O	1:B:196:PRO:HB2	1.93	0.68
1:B:100:SER:CB	1:B:103:LEU:HD12	2.24	0.68
1:A:256:SER:HB3	5:A:874:HOH:O	1.85	0.68
1:A:99:LEU:HD21	1:B:36:ILE:CD1	2.22	0.68
1:B:30:VAL:HG13	1:B:202:ARG:HD3	1.76	0.68
1:B:247:GLU:CD	1:B:314:GLN:HE21	1.97	0.68
1:B:302:THR:OG1	1:B:305:GLN:HG3	1.94	0.68
1:A:44:ARG:O	1:A:47:ASP:HB2	1.93	0.67
1:A:133:HIS:HA	1:A:184:HIS:CE1	2.28	0.67
1:A:182:MET:HB2	1:A:186:HIS:NE2	2.10	0.67
1:A:198:THR:HG21	1:B:328:GLY:O	1.94	0.67
1:A:170:VAL:HG22	1:A:189:MET:HG2	1.77	0.67
1:B:218:LEU:HB3	1:B:310:HIS:ND1	2.10	0.67
1:B:239:PRO:HD2	1:B:242:ALA:HB2	1.76	0.67
1:A:287:ASP:OD1	5:A:672:HOH:O	2.12	0.67
1:A:207:LYS:NZ	5:A:855:HOH:O	2.28	0.67
1:A:171:PHE:HB2	1:A:293:MET:HG3	1.76	0.67
1:A:186:HIS:NE2	3:A:601:AMP:P	2.66	0.67
1:B:337:PHE:HB3	1:B:339:GLU:OE1	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:235:VAL:O	1:A:235:VAL:HG13	1.94	0.67
1:B:76:GLU:HA	1:B:92:ILE:HG22	1.76	0.67
1:A:276:LEU:HG	1:A:277:MET:HE2	1.76	0.67
1:B:33:ARG:CG	1:B:33:ARG:NH1	2.53	0.67
1:A:118:ILE:HG13	1:B:25:LEU:HB2	1.77	0.67
1:A:171:PHE:CZ	1:B:325:PHE:HB2	2.29	0.67
1:B:178:ALA:HB1	1:B:291:ASN:OD1	1.94	0.67
1:A:61:SER:O	5:A:753:HOH:O	2.12	0.67
1:B:248:ILE:HD12	1:B:281:ILE:HD11	1.77	0.67
1:B:165:ILE:CG2	1:B:191:ALA:HB1	2.24	0.67
1:B:252:PRO:CG	1:B:310:HIS:HE2	2.02	0.67
1:B:260:HIS:ND1	5:B:618:HOH:O	2.27	0.67
1:A:67:ILE:HD11	1:A:86:ASN:HA	1.76	0.67
1:A:252:PRO:HG3	1:A:311:TRP:CD1	2.30	0.66
1:A:252:PRO:HG2	1:A:310:HIS:NE2	2.10	0.66
1:A:125:ASP:HB2	1:A:189:MET:HB2	1.76	0.66
1:A:76:GLU:HA	1:A:92:ILE:HG22	1.76	0.66
1:A:275:LYS:HD3	5:A:637:HOH:O	1.93	0.66
1:A:172:LYS:HG3	1:A:186:HIS:O	1.96	0.66
1:A:70:GLU:OE1	1:A:70:GLU:N	2.18	0.66
1:A:226:PHE:O	1:A:237:VAL:HB	1.95	0.66
1:A:351:THR:OXT	5:A:866:HOH:O	2.12	0.66
1:B:49:LYS:HB3	1:B:286:ASN:ND2	2.10	0.66
1:A:48:PHE:O	1:A:49:LYS:HD3	1.94	0.66
1:A:89:LEU:C	1:A:89:LEU:HD12	2.15	0.66
1:B:188:GLN:NE2	3:B:602:AMP:H5'2	2.11	0.66
1:A:129:GLU:HB2	1:A:185:SER:O	1.95	0.66
1:B:25:LEU:HD13	1:B:35:VAL:O	1.94	0.66
1:A:226:PHE:HE2	1:A:338:PRO:HG2	1.58	0.66
1:A:245:PRO:HA	1:A:334:ASN:HD21	1.59	0.66
1:B:196:PRO:HG2	1:B:199:VAL:CG2	2.25	0.66
1:A:127:VAL:HG11	1:A:152:TYR:CE1	2.31	0.66
1:B:292:TYR:HA	1:B:314:GLN:O	1.95	0.66
1:B:273:LEU:O	1:B:277:MET:HG2	1.96	0.66
1:B:27:LYS:HG3	1:B:33:ARG:O	1.95	0.66
1:B:239:PRO:HB2	1:B:242:ALA:HB2	1.77	0.66
1:A:341:VAL:O	1:A:345:MET:HG2	1.96	0.66
1:A:91:VAL:HG22	1:A:127:VAL:HG22	1.77	0.66
1:A:303:GLU:O	1:A:306:LEU:HB2	1.96	0.66
1:A:130:SER:OG	1:A:135:ILE:HD12	1.96	0.66
1:B:264:ASP:OD1	5:B:732:HOH:O	2.13	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:252:PRO:HG2	1:A:310:HIS:NE2	2.10	0.66
1:A:256:SER:HB3	5:A:875:HOH:O	1.95	0.66
1:A:117:THR:HG23	1:B:24:GLU:HG2	1.78	0.66
1:A:118:ILE:HG12	1:B:34:TRP:CZ3	2.31	0.66
1:A:332:TYR:HB3	5:A:644:HOH:O	1.96	0.66
1:A:174:GLN:HG3	1:A:290:TYR:CE1	2.31	0.66
1:B:172:LYS:HE3	1:B:174:GLN:HB2	1.76	0.65
1:A:197:PRO:HD2	1:B:329:THR:O	1.95	0.65
1:A:222:LYS:CG	1:A:235:VAL:HG21	2.25	0.65
1:A:170:VAL:CG1	1:A:294:ILE:HD12	2.26	0.65
1:A:346:ARG:HD2	5:A:878:HOH:O	1.94	0.65
1:A:148:ILE:HG22	1:A:152:TYR:CE2	2.31	0.65
1:A:186:HIS:NE2	3:A:601:AMP:P	2.69	0.65
1:A:106:GLN:NE2	5:A:721:HOH:O	2.28	0.65
1:B:130:SER:HB2	5:B:721:HOH:O	1.96	0.65
1:B:106:GLN:HG3	5:B:801:HOH:O	1.96	0.65
1:B:30:VAL:HG21	1:B:249:TRP:CH2	2.31	0.65
1:B:200:SER:OG	5:B:746:HOH:O	2.14	0.65
1:A:219:CYS:SG	1:A:220:GLU:N	2.69	0.65
1:A:51:LYS:CE	1:A:320:SER:HA	2.27	0.65
1:B:279:GLN:OE1	1:B:350:LEU:HD13	1.96	0.65
1:B:33:ARG:HH22	1:B:243:THR:HG1	1.40	0.65
1:B:279:GLN:HB3	1:B:350:LEU:HD13	1.79	0.65
1:A:174:GLN:C	1:A:174:GLN:NE2	2.50	0.65
1:A:170:VAL:HG11	1:A:294:ILE:HD12	1.77	0.65
1:A:78:PHE:CE1	1:A:154:LYS:HD3	2.32	0.65
1:A:334:ASN:C	1:A:334:ASN:HD22	2.00	0.65
1:B:94:ASN:O	5:B:698:HOH:O	2.15	0.65
1:B:213:THR:CB	1:B:215:LYS:HE2	2.27	0.65
1:A:310:HIS:HD2	1:A:311:TRP:O	1.80	0.65
1:A:186:HIS:CE1	3:A:601:AMP:P	2.89	0.65
1:B:77:LEU:HD13	1:B:155:ARG:CZ	2.26	0.65
1:B:295:HIS:ND1	5:B:644:HOH:O	2.29	0.65
1:A:195:VAL:HG13	1:A:199:VAL:HB	1.77	0.65
1:B:154:LYS:O	1:B:158:GLN:HG3	1.97	0.65
1:B:224:LYS:CE	1:B:224:LYS:HA	2.26	0.65
1:A:241:ALA:O	1:A:242:ALA:O	2.15	0.65
1:B:101:ARG:HH12	1:B:124:HIS:H	1.45	0.65
1:A:106:GLN:CB	1:A:119:VAL:HG11	2.27	0.65
1:B:344:VAL:O	1:B:348:VAL:HG23	1.96	0.65
1:B:25:LEU:HD22	1:B:36:ILE:HG23	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:33:ARG:HG3	1:B:33:ARG:HH11	1.60	0.65
1:A:74:ALA:HB3	1:A:93:GLU:O	1.97	0.65
1:B:76:GLU:OE1	5:B:714:HOH:O	2.15	0.65
1:B:67:ILE:O	1:B:67:ILE:HG23	1.97	0.65
1:A:93:GLU:OE1	5:A:664:HOH:O	2.15	0.65
1:B:236:SER:HA	1:B:250:ILE:HA	1.77	0.65
1:A:65:PHE:HE2	1:A:186:HIS:ND1	1.95	0.65
1:B:100:SER:HB3	1:B:103:LEU:HD12	1.79	0.65
1:B:252:PRO:HG3	1:B:311:TRP:NE1	2.12	0.65
1:A:252:PRO:HG2	1:A:310:HIS:CD2	2.32	0.65
1:A:25:LEU:HG	1:A:36:ILE:HA	1.78	0.65
1:A:23:PRO:O	1:B:120:GLY:HA3	1.98	0.64
1:A:350:LEU:HB2	5:A:819:HOH:O	1.97	0.64
1:A:34:TRP:O	1:A:331:CYS:SG	2.54	0.64
1:A:94:ASN:HB2	1:A:124:HIS:O	1.97	0.64
1:A:228:ILE:O	1:A:346:ARG:HG2	1.97	0.64
1:A:44:ARG:HG2	1:A:46:THR:HG22	1.79	0.64
3:B:602:AMP:H2'	5:B:683:HOH:O	1.97	0.64
1:A:49:LYS:HD2	1:A:286:ASN:ND2	2.12	0.64
1:B:335:PRO:O	1:B:336:VAL:HG23	1.97	0.64
1:A:169:GLN:HE21	1:A:293:MET:HB3	1.63	0.64
1:A:249:TRP:CB	1:A:251:ILE:HD11	2.27	0.64
1:B:90:ARG:CZ	5:B:794:HOH:O	2.45	0.64
1:B:219:CYS:SG	1:B:220:GLU:N	2.69	0.64
1:A:44:ARG:HG2	1:A:46:THR:HG22	1.79	0.64
1:A:179:GLY:O	3:A:601:AMP:O2P	2.15	0.64
1:A:305:GLN:HA	1:A:308:TYR:CZ	2.32	0.64
1:A:63:CYS:SG	1:A:65:PHE:N	2.67	0.64
1:A:118:ILE:O	1:A:118:ILE:HG13	1.98	0.64
1:A:136:GLN:HG2	1:A:139:ASP:CG	2.17	0.64
1:B:216:CYS:SG	1:B:255:HIS:CE1	2.90	0.64
1:B:27:LYS:HG3	1:B:33:ARG:H	1.63	0.64
1:A:130:SER:OG	1:A:131:PRO:HD2	1.98	0.64
1:A:256:SER:HB3	5:A:874:HOH:O	1.98	0.64
1:A:25:LEU:HB2	1:B:118:ILE:HG13	1.80	0.64
1:A:66:CYS:SG	1:A:133:HIS:HB2	2.37	0.64
1:A:194:VAL:HG21	1:B:34:TRP:CD1	2.33	0.64
1:B:182:MET:HG3	5:B:664:HOH:O	1.97	0.64
1:B:218:LEU:CB	1:B:310:HIS:ND1	2.61	0.64
1:B:237:VAL:N	1:B:249:TRP:O	2.27	0.64
1:B:346:ARG:NH1	1:B:346:ARG:CB	2.50	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:71:GLN:HE21	1:A:71:GLN:HA	1.62	0.64
1:A:67:ILE:HA	1:A:70:GLU:OE2	1.98	0.64
1:A:197:PRO:HG2	1:B:33:ARG:HB2	1.80	0.64
1:A:82:ASP:OD1	1:A:83:HIS:ND1	2.27	0.64
1:A:343:LYS:NZ	1:A:347:GLU:OE2	2.30	0.64
1:A:162:HIS:C	1:A:164:SER:N	2.49	0.64
1:A:237:VAL:HG23	1:A:238:ALA:N	2.13	0.64
1:A:168:ILE:HA	1:A:191:ALA:HA	1.78	0.64
1:B:176:ALA:N	5:B:643:HOH:O	2.30	0.64
1:A:143:VAL:HG13	5:A:786:HOH:O	1.98	0.64
1:B:132:VAL:HG11	1:B:135:ILE:HG12	1.78	0.64
1:B:127:VAL:O	1:B:186:HIS:CA	2.46	0.64
1:A:76:GLU:HA	1:A:92:ILE:HG22	1.80	0.64
1:A:254:ASP:HB2	5:A:645:HOH:O	1.98	0.64
1:A:24:GLU:CD	1:A:26:ARG:HE	2.01	0.64
1:A:127:VAL:O	1:A:187:SER:N	2.31	0.63
1:A:182:MET:HG2	3:A:601:AMP:H5'1	1.79	0.63
1:A:44:ARG:HG2	1:A:46:THR:HG22	1.80	0.63
1:A:216:CYS:HB2	1:A:308:TYR:HA	1.79	0.63
1:A:186:HIS:CD2	3:A:601:AMP:P	2.91	0.63
1:A:203:LEU:HD23	5:A:634:HOH:O	1.97	0.63
1:A:293:MET:O	1:A:313:LEU:HD12	1.97	0.63
1:A:170:VAL:HG22	1:A:189:MET:CE	2.27	0.63
1:B:132:VAL:HB	1:B:135:ILE:CD1	2.27	0.63
1:A:99:LEU:CD1	1:A:122:GLY:HA3	2.28	0.63
1:A:93:GLU:OE2	5:A:716:HOH:O	2.15	0.63
1:A:302:THR:OG1	1:A:305:GLN:HG3	1.99	0.63
1:B:171:PHE:HB2	1:B:293:MET:HE2	1.80	0.63
1:B:181:SER:H	3:B:602:AMP:P	2.21	0.63
1:A:25:LEU:HB2	1:B:118:ILE:HG12	1.79	0.63
1:B:320:SER:N	5:B:688:HOH:O	2.31	0.63
1:A:292:TYR:OH	1:A:294:ILE:HD11	1.99	0.63
1:B:135:ILE:HG23	1:B:139:ASP:HB2	1.79	0.63
1:A:341:VAL:O	1:A:345:MET:HG2	1.99	0.63
1:B:25:LEU:HD11	1:B:36:ILE:CG1	2.29	0.63
1:B:206:THR:HB	1:B:308:TYR:HB2	1.79	0.63
1:A:71:GLN:HG2	5:A:710:HOH:O	1.98	0.63
1:A:70:GLU:CD	1:A:70:GLU:H	2.02	0.63
1:A:104:GLU:HB2	5:A:819:HOH:O	1.97	0.63
1:B:178:ALA:HB1	1:B:291:ASN:ND2	2.13	0.63
1:B:26:ARG:O	1:B:35:VAL:HG12	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:256:SER:O	1:A:310:HIS:HA	1.98	0.63
1:A:82:ASP:OD1	1:A:83:HIS:ND1	2.32	0.63
1:A:87:TRP:CH2	1:A:131:PRO:HA	2.33	0.63
1:A:282:ALA:HB1	1:A:287:ASP:OD1	1.98	0.63
1:A:197:PRO:HG3	5:B:790:HOH:O	1.96	0.63
1:B:240:PHE:CA	1:B:338:PRO:HG3	2.29	0.63
1:B:203:LEU:O	1:B:206:THR:OG1	2.17	0.63
1:A:297:SER:HB2	1:A:309:THR:CG2	2.28	0.63
1:B:74:ALA:HB2	1:B:95:LEU:HB2	1.79	0.63
1:B:104:GLU:HB2	1:B:121:PHE:CE1	2.33	0.63
1:A:245:PRO:HA	4:A:607:EDO:O2	1.99	0.63
1:A:67:ILE:HG13	1:A:87:TRP:NE1	2.14	0.63
1:A:67:ILE:HD11	1:A:85:PRO:O	1.99	0.63
1:A:322:VAL:HB	1:A:326:GLU:CB	2.28	0.63
1:A:297:SER:HB2	1:A:309:THR:HG21	1.81	0.63
1:A:79:ARG:HH11	1:A:90:ARG:NH2	1.96	0.63
1:B:46:THR:CB	1:B:344:VAL:HG21	2.26	0.62
1:B:25:LEU:HD11	1:B:36:ILE:HG12	1.81	0.62
1:B:177:SER:O	1:B:318:GLN:NE2	2.32	0.62
1:B:101:ARG:HA	1:B:121:PHE:CE1	2.33	0.62
1:A:129:GLU:OE2	1:A:186:HIS:N	2.33	0.62
1:B:234:PHE:HB2	1:B:273:LEU:CD2	2.28	0.62
1:A:76:GLU:HA	1:A:92:ILE:CG2	2.20	0.62
1:A:213:THR:OG1	1:A:215:LYS:HG2	1.99	0.62
1:A:76:GLU:OE2	1:A:90:ARG:NH2	2.29	0.62
1:A:79:ARG:O	1:A:81:PRO:O	2.17	0.62
1:A:304:SER:O	1:A:307:PRO:HD2	1.99	0.62
1:A:79:ARG:HD3	1:A:87:TRP:HB3	1.81	0.62
1:B:136:GLN:NE2	1:B:174:GLN:HE22	1.97	0.62
1:B:178:ALA:HB2	1:B:318:GLN:HB2	1.80	0.62
1:A:82:ASP:OD1	1:A:83:HIS:ND1	2.28	0.62
1:B:231:SER:HB2	1:B:269:ASP:OD1	1.99	0.62
1:A:26:ARG:NH2	1:A:337:PHE:CD2	2.68	0.62
1:A:184:HIS:O	1:A:186:HIS:CD2	2.52	0.62
1:B:127:VAL:O	1:B:186:HIS:HA	1.98	0.62
1:A:335:PRO:HG2	1:A:336:VAL:HG23	1.79	0.62
1:B:186:HIS:CD2	3:B:602:AMP:H5'1	2.35	0.62
1:B:177:SER:OG	1:B:318:GLN:NE2	2.32	0.62
1:A:44:ARG:HG2	1:A:46:THR:HG22	1.80	0.62
1:B:193:PRO:O	1:B:194:VAL:HG13	2.00	0.62
1:A:197:PRO:HB2	1:B:330:GLY:HA3	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:247:GLU:OE1	1:B:314:GLN:NE2	2.32	0.62
1:B:278:LEU:HD22	1:B:290:TYR:CZ	2.35	0.62
1:A:242:ALA:HB3	4:A:607:EDO:H12	1.82	0.62
1:B:226:PHE:CE1	1:B:339:GLU:HG3	2.34	0.62
1:A:99:LEU:HD21	1:B:36:ILE:HD13	1.81	0.62
1:A:106:GLN:HG3	5:A:721:HOH:O	1.99	0.62
1:A:172:LYS:N	1:A:292:TYR:O	2.32	0.62
1:A:88:LYS:HE3	5:A:713:HOH:O	1.99	0.62
5:A:739:HOH:O	1:B:117:THR:HG22	1.99	0.62
1:B:106:GLN:O	1:B:107:SER:HB2	1.99	0.62
1:B:89:LEU:O	1:B:89:LEU:HD12	2.00	0.62
1:B:25:LEU:HD13	1:B:36:ILE:HG12	1.80	0.62
1:A:154:LYS:NZ	5:A:853:HOH:O	2.28	0.62
1:A:119:VAL:HG22	5:A:701:HOH:O	2.00	0.61
1:A:104:GLU:CB	5:A:819:HOH:O	2.48	0.61
1:B:32:ASN:CB	1:B:201:SER:HB3	2.29	0.61
1:B:90:ARG:NH2	5:B:794:HOH:O	2.33	0.61
1:A:127:VAL:O	1:A:186:HIS:HA	2.00	0.61
1:B:281:ILE:HG23	1:B:285:LEU:HD12	1.82	0.61
1:B:76:GLU:HB2	1:B:90:ARG:NH1	2.14	0.61
1:B:209:TYR:CE2	1:B:213:THR:HG21	2.35	0.61
1:A:27:LYS:HD2	1:A:34:TRP:CE2	2.34	0.61
1:A:237:VAL:O	1:A:248:ILE:HG23	2.01	0.61
1:A:236:SER:H	1:A:273:LEU:HD21	1.63	0.61
1:B:34:TRP:HB2	5:B:786:HOH:O	1.99	0.61
1:A:182:MET:HE1	5:A:759:HOH:O	2.00	0.61
1:A:231:SER:HB2	1:A:269:ASP:OD1	1.99	0.61
1:B:181:SER:O	1:B:182:MET:HG3	2.00	0.61
1:A:171:PHE:HE1	1:A:173:ASN:HD21	1.49	0.61
1:B:226:PHE:CE1	1:B:339:GLU:HG3	2.36	0.61
1:B:33:ARG:HD3	5:B:712:HOH:O	2.00	0.61
1:B:33:ARG:NH2	1:B:243:THR:OG1	2.24	0.61
1:B:224:LYS:O	1:B:240:PHE:HB2	2.00	0.61
1:A:150:ILE:HG21	5:A:786:HOH:O	2.00	0.61
1:B:106:GLN:O	1:B:107:SER:CB	2.48	0.61
1:A:27:LYS:HE2	1:A:32:ASN:C	2.21	0.61
1:A:343:LYS:NZ	1:A:347:GLU:OE2	2.32	0.61
1:B:154:LYS:NZ	5:B:833:HOH:O	2.25	0.61
1:B:180:ALA:HA	3:B:602:AMP:O2P	1.99	0.61
1:A:350:LEU:HB2	5:A:812:HOH:O	2.01	0.61
1:A:346:ARG:HD3	5:A:881:HOH:O	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:252:PRO:HG3	1:A:311:TRP:NE1	2.16	0.61
1:A:329:THR:O	1:B:198:THR:HG23	2.00	0.61
1:B:187:SER:HA	5:B:630:HOH:O	2.00	0.61
1:A:247:GLU:O	1:A:248:ILE:HD12	2.01	0.61
1:A:136:GLN:HG2	1:A:139:ASP:CG	2.21	0.61
1:B:266:LYS:NZ	5:B:663:HOH:O	2.27	0.61
1:A:84:ASP:OD1	1:A:85:PRO:HD2	2.01	0.61
1:B:74:ALA:HB3	1:B:93:GLU:O	2.01	0.61
1:B:106:GLN:O	1:B:119:VAL:HG21	2.01	0.61
1:B:63:CYS:SG	1:B:65:PHE:HB2	2.41	0.61
1:B:186:HIS:NE2	3:B:602:AMP:P	2.74	0.61
1:A:73:CYS:SG	1:A:90:ARG:NH1	2.74	0.61
1:B:226:PHE:CZ	1:B:339:GLU:HG3	2.36	0.61
1:A:325:PHE:HE1	1:B:190:MET:HG2	1.65	0.60
1:B:292:TYR:HA	1:B:314:GLN:O	2.01	0.60
1:B:168:ILE:CD1	1:B:299:LEU:HD11	2.32	0.60
1:A:68:GLY:H	1:A:70:GLU:CD	2.05	0.60
1:B:177:SER:OG	1:B:318:GLN:HG2	2.01	0.60
1:B:67:ILE:HG13	1:B:87:TRP:NE1	2.17	0.60
1:B:104:GLU:HB2	1:B:121:PHE:CE1	2.36	0.60
1:A:49:LYS:HB3	1:A:286:ASN:HD22	1.66	0.60
1:A:65:PHE:CD2	1:A:128:ILE:HG12	2.36	0.60
1:B:216:CYS:HB3	1:B:219:CYS:SG	2.41	0.60
1:B:231:SER:HB2	1:B:269:ASP:OD1	2.02	0.60
1:B:219:CYS:O	5:B:667:HOH:O	2.17	0.60
1:A:30:VAL:HG13	1:A:202:ARG:HD3	1.83	0.60
1:A:222:LYS:HE3	5:A:798:HOH:O	2.01	0.60
1:B:234:PHE:CE1	1:B:270:LEU:HB2	2.36	0.60
1:A:121:PHE:HE2	1:A:164:SER:OG	1.84	0.60
1:A:207:LYS:HE2	1:A:211:GLU:OE1	2.00	0.60
1:A:188:GLN:NE2	3:A:601:AMP:H5'2	2.17	0.60
1:B:89:LEU:C	1:B:89:LEU:HD12	2.21	0.60
1:B:281:ILE:HG23	1:B:285:LEU:HD12	1.84	0.60
1:B:256:SER:O	1:B:310:HIS:HA	2.00	0.60
1:B:154:LYS:O	1:B:157:ASN:HB2	2.00	0.60
1:A:100:SER:HB3	1:A:120:GLY:O	2.02	0.60
1:B:123:PHE:HB2	1:B:191:ALA:HB3	1.83	0.60
1:B:322:VAL:HB	1:B:326:GLU:CB	2.32	0.60
1:A:242:ALA:HB3	4:A:607:EDO:H12	1.83	0.60
1:A:285:LEU:HB2	1:A:288:PRO:HD3	1.82	0.60
1:B:50:SER:HB2	1:B:288:PRO:HB3	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:49:LYS:HE2	1:B:284:GLN:O	2.02	0.60
1:B:38:SER:O	1:B:335:PRO:HA	2.02	0.60
1:A:212:GLU:HG3	1:A:213:THR:HG23	1.82	0.60
1:A:165:ILE:CG2	1:A:191:ALA:HB1	2.32	0.60
1:B:171:PHE:HE2	1:B:190:MET:HB2	1.67	0.60
1:A:256:SER:HB3	5:A:876:HOH:O	2.00	0.60
1:A:256:SER:N	1:A:310:HIS:HD2	1.99	0.60
1:B:232:SER:OG	5:B:678:HOH:O	2.16	0.60
1:B:249:TRP:HA	1:B:313:LEU:O	2.01	0.60
1:A:27:LYS:HB2	1:A:34:TRP:CE3	2.37	0.60
1:B:171:PHE:CE2	1:B:190:MET:HB2	2.36	0.60
1:A:281:ILE:CD1	1:A:315:ILE:HG21	2.32	0.60
1:B:227:VAL:HG21	5:B:757:HOH:O	2.00	0.60
1:B:250:ILE:HD11	1:B:277:MET:CG	2.30	0.60
1:B:224:LYS:HE2	1:B:224:LYS:CA	2.29	0.60
1:A:65:PHE:HE2	1:A:126:VAL:HG11	1.67	0.60
1:A:92:ILE:HD13	1:A:128:ILE:HD11	1.83	0.60
1:B:250:ILE:HB	1:B:313:LEU:HB3	1.82	0.60
1:A:294:ILE:HB	5:A:617:HOH:O	2.01	0.60
1:B:240:PHE:HA	1:B:338:PRO:CG	2.30	0.60
1:A:249:TRP:CD1	1:A:314:GLN:HG3	2.36	0.60
1:A:319:LEU:O	1:A:320:SER:O	2.19	0.60
1:B:269:ASP:C	1:B:271:GLY:N	2.51	0.60
1:B:89:LEU:HD12	1:B:89:LEU:C	2.22	0.60
1:A:278:LEU:HD22	1:A:290:TYR:CZ	2.36	0.60
1:B:25:LEU:HD23	1:B:25:LEU:N	2.17	0.60
1:A:156:ILE:HG21	1:A:260:HIS:ND1	2.16	0.60
1:B:292:TYR:HB2	1:B:313:LEU:HD21	1.83	0.60
1:A:195:VAL:CG1	1:A:199:VAL:HB	2.31	0.60
1:A:89:LEU:HB2	1:A:128:ILE:O	2.01	0.60
1:A:239:PRO:HB2	1:A:242:ALA:HB2	1.84	0.60
1:A:246:PHE:HA	1:A:341:VAL:HG11	1.83	0.60
1:A:233:HIS:ND1	5:A:860:HOH:O	2.30	0.60
1:A:243:THR:HB	1:A:244:TYR:CD2	2.37	0.59
1:A:254:ASP:OD1	5:A:859:HOH:O	2.17	0.59
1:A:176:ALA:HA	1:A:180:ALA:O	2.02	0.59
1:B:180:ALA:HA	3:B:602:AMP:O2P	2.02	0.59
1:B:165:ILE:HG22	1:B:166:ASN:N	2.17	0.59
1:B:71:GLN:HB3	5:B:716:HOH:O	2.02	0.59
1:A:236:SER:HA	1:A:249:TRP:O	2.02	0.59
1:B:237:VAL:O	1:B:248:ILE:HA	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:169:GLN:OE1	1:B:329:THR:HG22	2.01	0.59
1:A:184:HIS:O	1:A:186:HIS:NE2	2.34	0.59
1:A:292:TYR:C	1:A:293:MET:SD	2.80	0.59
1:A:93:GLU:HA	1:A:125:ASP:OD1	2.02	0.59
1:A:171:PHE:CE2	1:B:325:PHE:HB2	2.37	0.59
1:A:106:GLN:CD	5:A:721:HOH:O	2.41	0.59
1:A:51:LYS:NZ	1:A:320:SER:HA	2.17	0.59
1:B:332:TYR:CD2	1:B:332:TYR:N	2.69	0.59
1:A:27:LYS:HD2	1:A:34:TRP:CE2	2.38	0.59
1:A:35:VAL:HG23	5:A:633:HOH:O	2.02	0.59
1:A:184:HIS:HB3	1:A:186:HIS:NE2	2.17	0.59
1:B:150:ILE:HD11	1:B:267:ALA:HB2	1.84	0.59
1:B:181:SER:O	1:B:182:MET:HE3	2.02	0.59
1:A:186:HIS:NE2	3:A:601:AMP:H5'1	2.17	0.59
1:B:87:TRP:CE3	1:B:90:ARG:HG3	2.37	0.59
1:B:185:SER:HB2	5:B:693:HOH:O	2.02	0.59
1:A:124:HIS:CD2	1:A:190:MET:HG2	2.37	0.59
1:A:297:SER:HB2	1:A:309:THR:HG21	1.84	0.59
1:B:285:LEU:O	1:B:288:PRO:HD3	2.03	0.59
1:B:31:THR:HB	1:B:33:ARG:HG2	1.85	0.59
1:A:197:PRO:HB2	1:B:330:GLY:HA3	1.85	0.59
1:B:33:ARG:NH2	1:B:243:THR:OG1	2.35	0.59
1:A:213:THR:CB	1:A:215:LYS:HE3	2.32	0.59
1:B:341:VAL:HG21	4:B:610:EDO:O1	2.02	0.59
1:A:219:CYS:CB	1:A:310:HIS:CE1	2.80	0.59
1:A:169:GLN:O	1:A:189:MET:HA	2.02	0.59
1:B:326:GLU:C	1:B:328:GLY:H	2.05	0.59
1:B:341:VAL:O	1:B:345:MET:HG2	2.02	0.59
1:B:318:GLN:O	1:B:319:LEU:HD23	2.03	0.59
1:B:119:VAL:HG22	5:B:788:HOH:O	2.03	0.59
1:B:48:PHE:HB2	1:B:246:PHE:CE1	2.37	0.59
1:A:79:ARG:HH11	1:A:90:ARG:HH21	1.50	0.59
1:B:31:THR:HG22	4:B:611:EDO:C1	2.31	0.59
1:B:154:LYS:O	1:B:158:GLN:HG3	2.03	0.59
1:A:250:ILE:HB	1:A:313:LEU:HB3	1.83	0.59
1:B:202:ARG:NE	5:B:651:HOH:O	2.23	0.59
1:B:76:GLU:N	5:B:796:HOH:O	2.36	0.59
1:A:25:LEU:CB	1:B:118:ILE:HD11	2.32	0.59
1:A:116:ARG:HH21	1:A:117:THR:N	1.97	0.59
1:B:106:GLN:HG3	5:B:803:HOH:O	2.02	0.59
1:B:342:ALA:O	1:B:346:ARG:HG3	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:204:ASP:OD2	5:A:798:HOH:O	2.17	0.59
1:B:71:GLN:CB	5:B:716:HOH:O	2.50	0.59
1:B:265:VAL:HG13	5:B:652:HOH:O	2.02	0.59
1:B:50:SER:HB2	1:B:288:PRO:HB3	1.84	0.59
1:B:323:GLY:O	1:B:327:ILE:HG13	2.03	0.59
1:A:129:GLU:HG3	1:A:186:HIS:HA	1.85	0.59
1:A:346:ARG:O	5:A:868:HOH:O	2.16	0.59
1:A:100:SER:O	1:A:121:PHE:HA	2.03	0.59
1:B:323:GLY:O	1:B:327:ILE:HG13	2.03	0.59
1:A:177:SER:C	1:A:318:GLN:HE22	2.06	0.59
1:B:196:PRO:HB2	1:B:197:PRO:HD2	1.85	0.59
1:A:245:PRO:HB3	1:A:335:PRO:HD2	1.83	0.59
1:B:292:TYR:HB2	1:B:315:ILE:HG12	1.85	0.58
1:A:46:THR:O	1:A:49:LYS:HE2	2.03	0.58
1:B:185:SER:HA	5:B:719:HOH:O	2.02	0.58
1:A:237:VAL:O	1:A:248:ILE:HG23	2.03	0.58
1:A:216:CYS:CB	1:A:219:CYS:HG	2.15	0.58
1:B:250:ILE:C	1:B:251:ILE:HG13	2.24	0.58
1:B:160:ALA:HA	1:B:299:LEU:HD13	1.84	0.58
1:A:73:CYS:HB3	3:A:601:AMP:N1	2.18	0.58
1:B:280:LYS:CG	1:B:350:LEU:HD11	2.34	0.58
1:B:343:LYS:O	1:B:347:GLU:HG2	2.03	0.58
1:B:250:ILE:CD1	1:B:277:MET:HG3	2.29	0.58
1:A:245:PRO:HB2	1:A:319:LEU:HD12	1.86	0.58
1:A:204:ASP:OD1	5:A:816:HOH:O	2.17	0.58
1:A:149:LEU:HD11	1:A:270:LEU:HD23	1.85	0.58
1:A:186:HIS:CE1	3:A:601:AMP:P	2.97	0.58
1:A:23:PRO:HG2	1:B:120:GLY:HA3	1.85	0.58
1:A:27:LYS:HB2	1:A:34:TRP:CE3	2.38	0.58
1:B:326:GLU:O	1:B:328:GLY:N	2.36	0.58
1:A:228:ILE:HG22	1:A:229:ASP:OD2	2.04	0.58
1:A:25:LEU:HB2	1:B:118:ILE:HD11	1.85	0.58
1:A:225:HIS:HB3	1:A:237:VAL:HG21	1.86	0.58
1:A:100:SER:HB3	1:A:103:LEU:HD12	1.84	0.58
1:A:210:PHE:O	1:A:214:GLY:N	2.35	0.58
1:A:216:CYS:HA	5:A:631:HOH:O	2.02	0.58
1:A:176:ALA:HA	1:A:180:ALA:O	2.03	0.58
1:B:231:SER:HB2	1:B:269:ASP:CG	2.24	0.58
1:B:232:SER:O	1:B:233:HIS:ND1	2.35	0.58
1:B:165:ILE:HG21	1:B:191:ALA:HB1	1.84	0.58
1:B:186:HIS:CE1	3:B:602:AMP:P	2.96	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:254:ASP:HB3	5:A:860:HOH:O	2.03	0.58
1:A:341:VAL:O	1:A:345:MET:HG2	2.04	0.58
1:B:32:ASN:HD22	1:B:205:GLY:N	2.02	0.58
1:B:25:LEU:HD12	1:B:34:TRP:HB3	1.85	0.58
1:B:252:PRO:HG3	1:B:311:TRP:CD1	2.38	0.58
1:B:186:HIS:CE1	3:B:602:AMP:P	2.95	0.58
1:B:172:LYS:CE	1:B:174:GLN:HB2	2.29	0.58
1:A:25:LEU:HB2	1:B:118:ILE:CG1	2.34	0.58
1:A:78:PHE:CE1	1:A:154:LYS:HD3	2.39	0.58
1:B:228:ILE:HG12	1:B:342:ALA:HA	1.86	0.58
1:B:149:LEU:HB3	1:B:262:LEU:HD21	1.84	0.58
1:A:228:ILE:HG13	1:A:237:VAL:HA	1.86	0.58
1:A:149:LEU:HB3	1:A:262:LEU:HD21	1.86	0.58
1:B:67:ILE:HG23	1:B:67:ILE:O	2.03	0.58
1:A:51:LYS:NZ	1:A:320:SER:HA	2.18	0.58
1:A:281:ILE:HG23	1:A:285:LEU:HD12	1.84	0.58
1:B:100:SER:N	1:B:120:GLY:O	2.34	0.58
1:B:217:CYS:HA	1:B:220:GLU:HG2	1.85	0.58
1:B:50:SER:HB2	1:B:288:PRO:HB3	1.85	0.58
1:B:252:PRO:HG3	1:B:256:SER:HB2	1.84	0.58
1:A:82:ASP:OD1	1:A:83:HIS:ND1	2.35	0.58
1:B:167:TYR:C	1:B:168:ILE:HG13	2.25	0.58
1:A:33:ARG:HD2	5:A:633:HOH:O	2.04	0.58
1:B:70:GLU:HA	5:B:714:HOH:O	2.03	0.58
1:B:155:ARG:CA	1:B:158:GLN:OE1	2.39	0.58
1:A:256:SER:CB	5:A:876:HOH:O	2.52	0.58
1:A:36:ILE:HD13	1:B:99:LEU:HD21	1.86	0.58
1:B:202:ARG:NH2	5:B:651:HOH:O	2.28	0.58
1:B:63:CYS:HB2	1:B:64:PRO:CD	2.33	0.58
1:B:274:LEU:HD13	1:B:313:LEU:HD11	1.86	0.58
1:A:186:HIS:HE1	3:A:601:AMP:P	2.24	0.58
1:B:153:LYS:HG2	1:B:157:ASN:HD21	1.69	0.57
1:B:255:HIS:CE1	1:B:307:PRO:O	2.56	0.57
1:B:81:PRO:HB2	1:B:84:ASP:HB2	1.86	0.57
1:A:249:TRP:CD1	1:A:314:GLN:HG3	2.39	0.57
1:A:87:TRP:CE3	1:A:90:ARG:HG3	2.39	0.57
1:B:75:PRO:HD2	1:B:93:GLU:OE2	2.04	0.57
1:B:246:PHE:HD2	1:B:285:LEU:HD11	1.69	0.57
1:A:25:LEU:HB2	1:B:118:ILE:CG1	2.35	0.57
1:A:153:LYS:HG3	1:A:260:HIS:HB2	1.86	0.57
1:A:313:LEU:C	1:A:313:LEU:HD23	2.24	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:76:GLU:HB2	1:A:90:ARG:NH2	2.19	0.57
1:B:101:ARG:CZ	5:B:698:HOH:O	2.52	0.57
1:A:305:GLN:HA	1:A:308:TYR:CE1	2.38	0.57
1:B:178:ALA:HB1	1:B:291:ASN:HD21	1.69	0.57
1:B:101:ARG:HD2	5:B:719:HOH:O	2.04	0.57
1:A:156:ILE:HG13	1:A:189:MET:HE1	1.86	0.57
1:A:182:MET:HB2	1:A:186:HIS:CE1	2.39	0.57
1:A:325:PHE:CE1	1:B:192:LEU:HD11	2.39	0.57
1:B:327:ILE:HG22	1:B:327:ILE:O	2.04	0.57
1:A:156:ILE:HG13	1:A:189:MET:HE3	1.85	0.57
1:A:25:LEU:HD11	1:B:99:LEU:HD21	1.86	0.57
1:A:90:ARG:NH1	5:A:708:HOH:O	2.34	0.57
1:A:73:CYS:HB3	1:A:92:ILE:HD12	1.86	0.57
1:A:194:VAL:HG11	1:B:34:TRP:CE2	2.39	0.57
1:B:346:ARG:HH11	1:B:346:ARG:HB3	1.67	0.57
1:A:45:PRO:HA	1:A:48:PHE:HE2	1.69	0.57
1:A:170:VAL:HG22	1:A:189:MET:CE	2.33	0.57
1:A:240:PHE:HA	1:A:338:PRO:HG3	1.87	0.57
1:A:22:SER:HB3	5:B:786:HOH:O	2.04	0.57
1:B:276:LEU:O	1:B:280:LYS:HG3	2.03	0.57
1:B:33:ARG:NH2	1:B:243:THR:OG1	2.36	0.57
1:A:306:LEU:HB2	1:A:307:PRO:HD3	1.85	0.57
1:A:198:THR:HG23	1:B:330:GLY:HA3	1.87	0.57
1:A:194:VAL:HB	5:A:744:HOH:O	2.05	0.57
1:B:305:GLN:HA	1:B:308:TYR:CZ	2.40	0.57
1:A:217:CYS:HB2	5:A:877:HOH:O	2.04	0.57
1:B:156:ILE:HG12	1:B:168:ILE:HD13	1.87	0.57
1:A:318:GLN:HA	4:A:609:EDO:H22	1.86	0.57
1:B:107:SER:HB2	1:B:119:VAL:HG22	1.87	0.57
1:A:67:ILE:HD12	1:A:87:TRP:O	2.05	0.57
1:B:121:PHE:HE2	1:B:164:SER:HB2	1.69	0.57
1:A:44:ARG:HG2	1:A:46:THR:HG22	1.85	0.57
1:A:305:GLN:HA	1:A:308:TYR:CZ	2.40	0.57
1:A:127:VAL:HG21	1:A:152:TYR:CE1	2.40	0.57
1:B:185:SER:HA	5:B:716:HOH:O	2.05	0.57
1:A:25:LEU:HD13	1:B:118:ILE:CD1	2.33	0.57
1:A:209:TYR:CD1	1:A:217:CYS:HB3	2.39	0.57
1:A:283:LYS:HD2	1:A:350:LEU:HD23	1.86	0.57
1:A:82:ASP:O	1:A:83:HIS:HB2	2.04	0.57
1:B:226:PHE:HB2	1:B:238:ALA:HB3	1.87	0.57
1:B:318:GLN:HG3	4:B:612:EDO:O2	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:213:THR:HB	1:B:215:LYS:HD2	1.87	0.57
1:B:232:SER:O	1:B:233:HIS:CG	2.58	0.57
1:A:276:LEU:O	1:A:280:LYS:HG3	2.05	0.57
1:A:44:ARG:HG3	1:A:45:PRO:HD2	1.87	0.57
1:B:136:GLN:HB2	1:B:139:ASP:HB2	1.85	0.57
1:B:104:GLU:HA	1:B:121:PHE:CD1	2.39	0.57
1:B:317:PRO:HB2	1:B:319:LEU:HG	1.87	0.57
1:B:121:PHE:CE2	1:B:164:SER:HB2	2.40	0.57
1:A:94:ASN:OD1	3:A:601:AMP:H1'	2.05	0.57
1:B:291:ASN:HB3	1:B:293:MET:CE	2.34	0.57
1:B:69:ARG:HB2	5:B:715:HOH:O	2.04	0.57
1:B:37:PHE:CE1	1:B:338:PRO:HD3	2.39	0.57
1:A:124:HIS:CG	1:A:190:MET:SD	2.98	0.57
1:A:172:LYS:O	1:A:291:ASN:HA	2.05	0.57
1:B:152:TYR:O	1:B:156:ILE:HG13	2.03	0.57
1:A:37:PHE:HA	1:A:334:ASN:O	2.05	0.57
1:A:44:ARG:HG2	1:A:46:THR:HG22	1.87	0.57
1:A:117:THR:OG1	1:B:24:GLU:CG	2.53	0.57
1:B:216:CYS:O	1:B:219:CYS:SG	2.61	0.57
1:A:324:GLY:N	1:B:291:ASN:ND2	2.49	0.56
1:B:226:PHE:CE1	1:B:339:GLU:HG3	2.40	0.56
1:A:165:ILE:HD12	1:A:191:ALA:HB1	1.86	0.56
1:B:345:MET:HA	1:B:348:VAL:HG23	1.86	0.56
1:B:106:GLN:O	1:B:107:SER:CB	2.52	0.56
1:B:322:VAL:HG12	1:B:326:GLU:HG2	1.86	0.56
1:A:69:ARG:HA	5:A:817:HOH:O	2.03	0.56
1:B:36:ILE:CG2	1:B:37:PHE:N	2.68	0.56
1:B:63:CYS:SG	1:B:133:HIS:CE1	2.98	0.56
1:A:234:PHE:CE1	1:A:270:LEU:HB2	2.39	0.56
1:A:336:VAL:CG1	1:A:341:VAL:HG23	2.34	0.56
1:B:226:PHE:HB3	1:B:342:ALA:HB2	1.87	0.56
1:B:154:LYS:NZ	5:B:836:HOH:O	2.37	0.56
1:A:145:ILE:HD12	1:A:275:LYS:HB2	1.87	0.56
1:A:145:ILE:CD1	1:A:275:LYS:HB2	2.35	0.56
1:B:226:PHE:CE1	1:B:339:GLU:HG3	2.40	0.56
1:B:145:ILE:HD11	1:B:275:LYS:HB2	1.87	0.56
1:A:234:PHE:HA	1:A:251:ILE:O	2.05	0.56
1:B:244:TYR:HB3	1:B:245:PRO:HD2	1.86	0.56
1:B:76:GLU:N	5:B:798:HOH:O	2.38	0.56
1:A:88:LYS:HE3	5:A:715:HOH:O	2.05	0.56
1:A:65:PHE:CE2	1:A:182:MET:HG3	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:292:TYR:O	1:B:293:MET:CE	2.53	0.56
1:A:345:MET:HA	1:A:348:VAL:HG23	1.88	0.56
1:B:81:PRO:HB2	1:B:84:ASP:HB2	1.86	0.56
1:A:265:VAL:HG23	5:A:808:HOH:O	2.05	0.56
1:A:88:LYS:HA	1:A:131:PRO:HD3	1.86	0.56
1:A:88:LYS:HE2	5:A:713:HOH:O	2.04	0.56
1:B:82:ASP:O	1:B:84:ASP:N	2.39	0.56
1:A:224:LYS:O	1:A:240:PHE:HB2	2.05	0.56
1:A:129:GLU:CG	1:A:186:HIS:HA	2.36	0.56
1:B:165:ILE:HG13	1:B:191:ALA:HB1	1.87	0.56
1:B:87:TRP:CE3	1:B:90:ARG:HG3	2.39	0.56
1:A:106:GLN:HB3	1:A:119:VAL:HG11	1.87	0.56
1:B:130:SER:O	1:B:184:HIS:NE2	2.35	0.56
1:B:165:ILE:HG23	1:B:191:ALA:HB1	1.87	0.56
1:A:90:ARG:NE	5:A:708:HOH:O	2.18	0.56
1:A:207:LYS:O	1:A:210:PHE:N	2.39	0.56
1:A:74:ALA:HB3	1:A:93:GLU:O	2.06	0.56
1:B:74:ALA:HB3	1:B:93:GLU:O	2.05	0.56
1:B:256:SER:HA	5:B:765:HOH:O	2.03	0.56
1:A:305:GLN:HA	1:A:308:TYR:CZ	2.41	0.56
1:A:302:THR:HG23	1:A:305:GLN:OE1	2.06	0.56
1:A:246:PHE:CD2	1:A:341:VAL:HG22	2.41	0.56
1:A:141:ASP:HB2	1:A:142:PRO:HD2	1.87	0.56
1:A:283:LYS:NZ	1:A:349:SER:O	2.39	0.56
1:B:48:PHE:O	1:B:319:LEU:HD22	2.04	0.56
1:B:226:PHE:CZ	1:B:339:GLU:HG3	2.41	0.56
1:A:89:LEU:HB2	1:A:128:ILE:O	2.06	0.56
3:B:602:AMP:H2'	5:B:685:HOH:O	2.06	0.56
1:B:66:CYS:O	5:B:715:HOH:O	2.17	0.56
1:B:157:ASN:O	1:B:161:GLN:HG3	2.06	0.56
1:B:234:PHE:CE1	1:B:270:LEU:HB2	2.41	0.56
1:B:232:SER:C	1:B:233:HIS:CG	2.78	0.56
1:A:225:HIS:CE1	1:A:240:PHE:H	2.21	0.56
1:A:216:CYS:HB3	1:A:219:CYS:SG	2.45	0.56
1:B:37:PHE:CZ	1:B:338:PRO:HD3	2.41	0.56
1:B:143:VAL:HG12	5:B:722:HOH:O	2.05	0.56
1:B:21:GLN:HG2	1:B:22:SER:H	1.71	0.56
1:A:219:CYS:SG	1:A:219:CYS:O	2.63	0.56
1:A:27:LYS:HD2	1:A:34:TRP:CZ2	2.41	0.56
1:A:27:LYS:HB2	1:A:34:TRP:CZ3	2.40	0.56
1:A:31:THR:HA	5:A:668:HOH:O	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:132:VAL:CG1	1:B:135:ILE:HG13	2.35	0.56
1:B:101:ARG:NH2	1:B:123:PHE:CD1	2.74	0.56
1:B:26:ARG:O	1:B:35:VAL:HG12	2.06	0.56
1:A:303:GLU:HA	1:A:306:LEU:HG	1.87	0.56
1:B:203:LEU:HD13	1:B:305:GLN:NE2	2.21	0.56
1:B:256:SER:C	1:B:258:HIS:H	2.08	0.56
1:A:263:ASP:OD1	1:A:266:LYS:HG3	2.06	0.56
1:B:226:PHE:CZ	1:B:339:GLU:HG3	2.40	0.56
1:B:170:VAL:HG22	1:B:189:MET:HG2	1.88	0.56
1:A:129:GLU:HG3	1:A:186:HIS:HA	1.88	0.56
1:B:173:ASN:OD1	1:B:291:ASN:ND2	2.39	0.56
1:A:215:LYS:HD2	1:A:220:GLU:CD	2.26	0.56
1:B:165:ILE:O	1:B:299:LEU:HD12	2.06	0.55
1:A:74:ALA:HB3	1:A:93:GLU:O	2.06	0.55
1:A:247:GLU:HG3	1:A:316:VAL:HG22	1.88	0.55
1:B:186:HIS:HD2	5:B:723:HOH:O	1.88	0.55
1:B:25:LEU:CD1	1:B:36:ILE:HG12	2.36	0.55
1:B:32:ASN:HB2	1:B:205:GLY:HA3	1.88	0.55
1:B:48:PHE:CE1	1:B:336:VAL:HG22	2.41	0.55
1:A:178:ALA:O	1:A:291:ASN:ND2	2.36	0.55
1:B:215:LYS:HE3	1:B:220:GLU:OE1	2.06	0.55
1:B:242:ALA:CB	4:B:610:EDO:H11	2.37	0.55
1:A:28:ASP:O	1:A:30:VAL:N	2.39	0.55
1:B:27:LYS:HE3	1:B:33:ARG:HA	1.87	0.55
1:B:101:ARG:HB2	1:B:123:PHE:CE1	2.40	0.55
1:A:132:VAL:HB	1:A:135:ILE:HD12	1.89	0.55
1:B:227:VAL:HG23	5:B:755:HOH:O	2.06	0.55
1:A:250:ILE:HD11	1:A:277:MET:HG3	1.88	0.55
1:A:228:ILE:CG1	1:A:342:ALA:HA	2.35	0.55
1:A:254:ASP:CB	5:A:645:HOH:O	2.55	0.55
1:A:39:PRO:HA	1:A:335:PRO:O	2.07	0.55
1:B:155:ARG:O	1:B:159:ILE:HG13	2.05	0.55
1:B:26:ARG:HH12	1:B:338:PRO:HG2	1.69	0.55
1:B:218:LEU:HD22	1:B:251:ILE:HD13	1.88	0.55
1:A:50:SER:CB	1:A:288:PRO:HB3	2.37	0.55
1:A:75:PRO:O	1:A:92:ILE:HB	2.06	0.55
1:B:196:PRO:HG2	1:B:199:VAL:HG21	1.88	0.55
1:B:48:PHE:CB	1:B:336:VAL:HG21	2.32	0.55
1:B:29:PRO:HB2	1:B:217:CYS:SG	2.47	0.55
1:A:87:TRP:HE3	1:A:89:LEU:N	2.05	0.55
1:A:71:GLN:HG2	5:A:710:HOH:O	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:129:GLU:OE2	1:B:137:LEU:HD13	2.06	0.55
1:A:82:ASP:OD1	1:A:83:HIS:ND1	2.34	0.55
1:A:167:TYR:CE2	1:A:296:THR:O	2.57	0.55
1:B:228:ILE:HG13	1:B:237:VAL:HA	1.89	0.55
1:A:147:ASP:O	1:A:150:ILE:N	2.40	0.55
1:A:72:GLU:HG2	5:A:772:HOH:O	2.06	0.55
1:B:325:PHE:HB3	5:B:631:HOH:O	2.05	0.55
1:B:313:LEU:HD23	1:B:314:GLN:N	2.21	0.55
1:A:216:CYS:CB	1:A:219:CYS:HB3	2.35	0.55
1:A:173:ASN:OD1	1:A:291:ASN:ND2	2.39	0.55
1:B:216:CYS:HB3	1:B:219:CYS:HB2	1.89	0.55
1:A:242:ALA:CB	4:A:607:EDO:H12	2.37	0.55
1:A:336:VAL:HG13	5:A:817:HOH:O	2.06	0.55
1:B:226:PHE:CZ	1:B:339:GLU:HG3	2.42	0.55
1:B:100:SER:N	1:B:120:GLY:O	2.30	0.55
1:A:87:TRP:CD2	1:A:90:ARG:HG3	2.42	0.55
1:B:258:HIS:HB3	1:B:260:HIS:CE1	2.42	0.55
1:A:67:ILE:HD12	1:A:131:PRO:CB	2.36	0.55
1:A:251:ILE:HG13	1:A:312:PHE:CB	2.36	0.55
1:B:246:PHE:CE1	1:B:341:VAL:HG22	2.41	0.55
1:A:39:PRO:CG	1:A:337:PHE:HE1	2.20	0.55
1:B:206:THR:HA	1:B:217:CYS:SG	2.47	0.55
1:B:88:LYS:HD2	5:B:800:HOH:O	2.06	0.55
1:B:25:LEU:HD22	1:B:36:ILE:HA	1.89	0.55
1:A:63:CYS:O	1:A:66:CYS:HB2	2.06	0.55
1:B:143:VAL:HA	1:B:268:VAL:CG1	2.35	0.55
1:A:203:LEU:HD23	5:A:634:HOH:O	2.05	0.55
1:A:184:HIS:HB2	5:A:630:HOH:O	2.07	0.55
1:A:71:GLN:NE2	1:A:71:GLN:HA	2.22	0.55
1:A:44:ARG:HB3	1:A:47:ASP:CG	2.27	0.55
1:A:37:PHE:CZ	1:A:338:PRO:HD3	2.41	0.55
1:B:21:GLN:NE2	5:B:765:HOH:O	2.39	0.55
1:B:177:SER:C	1:B:318:GLN:NE2	2.59	0.55
1:A:346:ARG:CD	5:A:878:HOH:O	2.53	0.55
1:A:218:LEU:HA	1:A:221:ALA:HB2	1.88	0.55
1:A:338:PRO:HG2	1:A:339:GLU:OE1	2.07	0.55
1:A:250:ILE:HG23	1:A:273:LEU:HD23	1.88	0.55
1:A:173:ASN:HA	1:A:291:ASN:ND2	2.21	0.55
1:A:25:LEU:HB2	1:B:118:ILE:CD1	2.36	0.55
1:A:106:GLN:O	1:A:107:SER:HB2	2.07	0.54
1:B:132:VAL:CG1	1:B:135:ILE:HG12	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:101:ARG:HB3	5:B:720:HOH:O	2.06	0.54
1:B:101:ARG:NH2	5:B:699:HOH:O	2.38	0.54
1:A:226:PHE:CZ	1:A:339:GLU:HG3	2.42	0.54
1:A:197:PRO:HG2	1:B:330:GLY:O	2.07	0.54
1:B:124:HIS:NE2	1:B:188:GLN:OE1	2.39	0.54
1:A:326:GLU:HG3	1:A:332:TYR:HA	1.88	0.54
1:A:123:PHE:H	1:A:191:ALA:HB3	1.71	0.54
1:B:301:VAL:HG22	1:B:305:GLN:HB2	1.89	0.54
1:B:323:GLY:O	1:B:326:GLU:HB2	2.07	0.54
1:A:169:GLN:HG2	1:B:329:THR:HG23	1.89	0.54
1:B:25:LEU:CD2	1:B:36:ILE:HD13	2.35	0.54
1:B:262:LEU:HD11	1:B:267:ALA:N	2.22	0.54
1:A:116:ARG:CZ	5:A:866:HOH:O	2.55	0.54
1:A:127:VAL:CG1	1:A:187:SER:HB2	2.38	0.54
1:B:145:ILE:HD12	1:B:275:LYS:HB2	1.90	0.54
1:A:206:THR:HG22	1:A:217:CYS:SG	2.47	0.54
1:B:165:ILE:O	1:B:299:LEU:HD12	2.06	0.54
1:A:278:LEU:O	1:A:281:ILE:N	2.40	0.54
1:B:228:ILE:CG1	1:B:342:ALA:HA	2.34	0.54
1:A:234:PHE:CA	1:A:253:LYS:HG3	2.38	0.54
1:B:306:LEU:HD22	5:B:654:HOH:O	2.08	0.54
1:A:226:PHE:CE1	1:A:339:GLU:HG3	2.42	0.54
1:A:239:PRO:HD2	1:A:242:ALA:HB2	1.89	0.54
1:A:104:GLU:HG3	1:A:121:PHE:CE1	2.43	0.54
1:B:207:LYS:HB2	1:B:308:TYR:CE2	2.43	0.54
1:A:132:VAL:HB	1:A:135:ILE:CD1	2.37	0.54
1:A:203:LEU:HD11	1:A:298:PRO:CG	2.37	0.54
1:B:48:PHE:HB2	1:B:336:VAL:CG2	2.33	0.54
1:B:33:ARG:HG3	1:B:33:ARG:NH1	2.22	0.54
1:A:161:GLN:NE2	5:A:788:HOH:O	2.39	0.54
1:A:126:VAL:HG21	3:A:601:AMP:O4'	2.07	0.54
1:A:165:ILE:HG22	1:A:299:LEU:CD1	2.38	0.54
1:A:273:LEU:O	1:A:274:LEU:C	2.43	0.54
1:A:216:CYS:HB3	1:A:219:CYS:SG	2.47	0.54
1:B:249:TRP:HA	1:B:313:LEU:O	2.08	0.54
5:A:739:HOH:O	1:B:117:THR:HG21	2.07	0.54
1:A:299:LEU:O	1:A:300:LYS:HD3	2.08	0.54
1:B:335:PRO:O	1:B:336:VAL:CG2	2.56	0.54
1:B:292:TYR:HA	1:B:314:GLN:O	2.08	0.54
1:B:132:VAL:O	1:B:184:HIS:CE1	2.60	0.54
1:B:155:ARG:O	1:B:159:ILE:HG13	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:254:ASP:CG	5:A:859:HOH:O	2.45	0.54
1:B:138:SER:O	1:B:279:GLN:NE2	2.41	0.54
1:A:229:ASP:HB2	1:A:277:MET:CE	2.38	0.54
1:A:104:GLU:HB3	5:A:687:HOH:O	2.08	0.54
1:A:147:ASP:OD2	5:A:787:HOH:O	2.18	0.54
1:A:218:LEU:HD22	1:A:251:ILE:HD13	1.89	0.54
1:A:192:LEU:HB3	1:A:193:PRO:HD2	1.89	0.54
1:B:149:LEU:HB3	1:B:262:LEU:CD2	2.38	0.54
1:A:197:PRO:O	1:A:201:SER:N	2.34	0.54
1:B:276:LEU:O	1:B:277:MET:C	2.47	0.54
1:A:239:PRO:O	1:A:338:PRO:HB3	2.08	0.54
1:A:99:LEU:CD2	1:B:25:LEU:HD21	2.36	0.54
1:B:101:ARG:NH1	1:B:125:ASP:OD1	2.41	0.54
1:A:161:GLN:CG	5:A:787:HOH:O	2.43	0.54
1:A:98:ALA:HB3	1:A:190:MET:HE1	1.90	0.54
1:A:52:SER:HB2	1:A:289:PRO:HG2	1.90	0.54
1:A:224:LYS:HB3	1:B:116:ARG:NH1	2.22	0.54
1:B:73:CYS:HA	3:B:602:AMP:HN62	1.73	0.54
1:B:186:HIS:ND1	3:B:602:AMP:P	2.81	0.54
1:B:123:PHE:CD2	1:B:159:ILE:HG23	2.42	0.54
1:B:37:PHE:HE1	1:B:336:VAL:O	1.91	0.53
1:A:230:GLU:HA	1:A:235:VAL:HA	1.91	0.53
1:A:169:GLN:NE2	1:B:329:THR:CG2	2.63	0.53
1:A:89:LEU:O	1:A:89:LEU:HD12	2.08	0.53
1:B:67:ILE:HD12	1:B:68:GLY:N	2.22	0.53
1:A:233:HIS:ND1	1:A:266:LYS:HE2	2.22	0.53
1:A:247:GLU:OE1	1:A:314:GLN:NE2	2.38	0.53
1:B:213:THR:HB	1:B:215:LYS:CD	2.38	0.53
5:A:682:HOH:O	1:B:198:THR:CG2	2.55	0.53
1:A:78:PHE:CZ	1:A:91:VAL:HG21	2.43	0.53
1:A:44:ARG:HB3	1:A:47:ASP:CG	2.29	0.53
1:B:145:ILE:CD1	1:B:275:LYS:HB2	2.38	0.53
1:A:146:GLY:HA2	1:A:267:ALA:O	2.07	0.53
1:B:173:ASN:ND2	1:B:291:ASN:HD21	2.05	0.53
1:B:276:LEU:CD1	5:B:769:HOH:O	2.56	0.53
1:B:182:MET:CE	1:B:182:MET:HA	2.38	0.53
1:A:101:ARG:C	1:A:103:LEU:H	2.11	0.53
1:B:206:THR:HG1	1:B:308:TYR:HD2	1.49	0.53
1:B:230:GLU:OE2	5:B:834:HOH:O	2.19	0.53
1:B:28:ASP:OD1	1:B:30:VAL:N	2.36	0.53
1:A:197:PRO:CD	5:B:785:HOH:O	2.56	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:280:LYS:NZ	5:A:866:HOH:O	2.37	0.53
1:B:305:GLN:HG2	1:B:308:TYR:OH	2.08	0.53
1:B:201:SER:O	1:B:202:ARG:C	2.47	0.53
1:B:150:ILE:HD11	1:B:267:ALA:HB2	1.90	0.53
1:A:218:LEU:O	1:A:221:ALA:HB2	2.08	0.53
1:B:252:PRO:CG	1:B:256:SER:HB2	2.37	0.53
1:A:26:ARG:O	1:A:34:TRP:HA	2.08	0.53
1:A:306:LEU:HB2	1:A:307:PRO:CD	2.38	0.53
1:A:30:VAL:HG13	1:A:202:ARG:HD3	1.89	0.53
1:A:330:GLY:O	1:B:197:PRO:HG2	2.08	0.53
1:A:213:THR:HB	1:A:215:LYS:HE2	1.88	0.53
1:B:28:ASP:OD1	1:B:30:VAL:HB	2.07	0.53
1:B:306:LEU:N	1:B:307:PRO:CD	2.72	0.53
1:A:22:SER:HB2	1:A:23:PRO:HD2	1.91	0.53
1:A:44:ARG:HE	1:A:47:ASP:CG	2.11	0.53
1:B:154:LYS:HE2	5:B:716:HOH:O	2.08	0.53
1:B:101:ARG:NH1	1:B:125:ASP:OD1	2.33	0.53
1:B:143:VAL:HG23	5:B:725:HOH:O	2.08	0.53
1:A:26:ARG:HD3	1:A:240:PHE:CE2	2.43	0.53
1:A:169:GLN:HE22	1:B:329:THR:HG23	1.69	0.53
1:A:28:ASP:HB2	1:A:241:ALA:CB	2.34	0.53
1:B:32:ASN:HD22	1:B:205:GLY:CA	2.21	0.53
1:A:137:LEU:HD21	1:A:292:TYR:OH	2.08	0.53
1:B:305:GLN:HG2	1:B:308:TYR:OH	2.09	0.53
1:B:290:TYR:HB3	1:B:317:PRO:HA	1.90	0.53
1:B:226:PHE:CZ	1:B:339:GLU:HG3	2.43	0.53
1:B:242:ALA:CB	4:B:610:EDO:H21	2.36	0.53
1:B:298:PRO:HD2	1:B:301:VAL:HB	1.89	0.53
1:B:101:ARG:HB3	1:B:101:ARG:CZ	2.38	0.53
1:A:251:ILE:HG13	1:A:312:PHE:HB2	1.90	0.53
1:B:145:ILE:HD12	1:B:275:LYS:HB2	1.91	0.53
1:A:293:MET:SD	1:B:327:ILE:HB	2.49	0.53
1:A:51:LYS:HE2	1:A:320:SER:HA	1.89	0.53
1:B:255:HIS:CE1	1:B:307:PRO:O	2.61	0.53
1:B:33:ARG:CD	5:B:705:HOH:O	2.35	0.53
1:A:140:ILE:HG22	1:A:145:ILE:HG13	1.91	0.53
1:B:68:GLY:O	1:B:69:ARG:HG2	2.09	0.53
1:B:101:ARG:NE	5:B:698:HOH:O	2.42	0.53
1:A:258:HIS:HB2	1:A:260:HIS:ND1	2.23	0.53
1:A:163:ASP:HA	5:A:728:HOH:O	2.08	0.53
1:B:200:SER:HB2	5:B:744:HOH:O	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:255:HIS:HA	1:A:310:HIS:ND1	2.22	0.53
1:A:149:LEU:HB3	1:A:262:LEU:CD2	2.38	0.53
1:A:78:PHE:CZ	1:A:91:VAL:HG21	2.44	0.53
1:A:247:GLU:OE1	1:A:314:GLN:NE2	2.38	0.53
1:A:93:GLU:OE2	5:A:714:HOH:O	2.19	0.53
1:A:297:SER:HB2	1:A:309:THR:CG2	2.39	0.53
1:A:28:ASP:CB	1:A:241:ALA:HB3	2.37	0.53
1:B:143:VAL:HG23	5:B:719:HOH:O	2.09	0.53
1:B:325:PHE:CE2	1:B:331:CYS:HB3	2.44	0.53
1:A:136:GLN:O	1:A:139:ASP:HB2	2.08	0.53
1:B:46:THR:HB	1:B:344:VAL:HG22	1.90	0.53
1:A:265:VAL:HG23	5:A:806:HOH:O	2.09	0.53
1:A:229:ASP:OD2	1:A:277:MET:HE1	2.09	0.53
1:A:174:GLN:HG3	1:A:290:TYR:CZ	2.44	0.53
1:A:94:ASN:OD1	3:A:601:AMP:H1'	2.09	0.52
1:A:229:ASP:CG	1:A:276:LEU:HD21	2.30	0.52
1:B:233:HIS:CG	1:B:266:LYS:HG2	2.44	0.52
1:A:154:LYS:HG2	1:A:158:GLN:NE2	2.25	0.52
1:B:246:PHE:HA	1:B:341:VAL:HG21	1.91	0.52
1:B:132:VAL:HG11	1:B:135:ILE:HG13	1.91	0.52
1:A:91:VAL:HG22	1:A:127:VAL:HG13	1.90	0.52
1:A:338:PRO:HA	4:A:607:EDO:H22	1.91	0.52
1:A:169:GLN:NE2	1:B:325:PHE:O	2.40	0.52
1:A:307:PRO:N	5:A:658:HOH:O	2.41	0.52
1:A:33:ARG:NH2	1:A:332:TYR:HE2	2.06	0.52
1:A:171:PHE:HA	1:A:293:MET:HA	1.92	0.52
1:A:233:HIS:CG	1:A:266:LYS:HE2	2.44	0.52
1:B:232:SER:N	1:B:269:ASP:OD1	2.31	0.52
1:B:252:PRO:HG2	1:B:310:HIS:NE2	2.24	0.52
1:B:209:TYR:OH	1:B:224:LYS:HE3	2.09	0.52
1:A:65:PHE:O	1:A:184:HIS:CE1	2.63	0.52
1:A:117:THR:HG23	1:B:26:ARG:CG	2.40	0.52
1:B:193:PRO:HG2	1:B:194:VAL:HG22	1.90	0.52
1:B:69:ARG:HD3	1:B:72:GLU:OE2	2.08	0.52
1:A:174:GLN:NE2	1:A:174:GLN:CA	2.71	0.52
1:A:345:MET:O	1:A:348:VAL:HG23	2.10	0.52
1:A:328:GLY:HA3	1:B:169:GLN:NE2	2.25	0.52
1:A:65:PHE:CE2	1:A:182:MET:HG3	2.44	0.52
1:B:63:CYS:HB3	1:B:133:HIS:CE1	2.44	0.52
1:B:26:ARG:HD2	1:B:37:PHE:CE2	2.44	0.52
1:B:245:PRO:O	1:B:317:PRO:HD2	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:209:TYR:CE2	1:A:213:THR:HG21	2.44	0.52
1:A:287:ASP:OD1	5:A:670:HOH:O	2.19	0.52
1:A:290:TYR:CB	1:A:317:PRO:HA	2.40	0.52
1:A:322:VAL:HB	1:A:326:GLU:OE2	2.10	0.52
1:A:286:ASN:OD1	5:A:749:HOH:O	2.19	0.52
1:B:264:ASP:HB3	5:B:672:HOH:O	2.08	0.52
1:A:121:PHE:HZ	1:A:164:SER:HB3	1.72	0.52
1:A:209:TYR:CE2	1:A:213:THR:HG21	2.45	0.52
1:A:169:GLN:HE22	1:B:328:GLY:C	2.10	0.52
1:B:226:PHE:CZ	1:B:339:GLU:HG3	2.45	0.52
1:A:28:ASP:CG	5:A:623:HOH:O	2.48	0.52
1:A:227:VAL:HA	1:A:237:VAL:CG1	2.36	0.52
1:A:170:VAL:HG22	1:A:189:MET:HE3	1.91	0.52
1:B:91:VAL:HG22	1:B:127:VAL:HG22	1.90	0.52
1:A:293:MET:N	1:A:293:MET:SD	2.82	0.52
1:B:226:PHE:CZ	1:B:339:GLU:HG3	2.44	0.52
1:B:33:ARG:HH22	1:B:243:THR:HG21	1.75	0.52
1:B:100:SER:HB3	1:B:103:LEU:CD1	2.39	0.52
1:A:186:HIS:NE2	3:A:601:AMP:H5'2	2.25	0.52
1:A:180:ALA:HA	3:A:601:AMP:O2P	2.09	0.52
1:A:281:ILE:HG23	1:A:285:LEU:CD1	2.34	0.52
1:A:101:ARG:O	1:A:103:LEU:N	2.38	0.52
1:B:276:LEU:HG	1:B:280:LYS:HE3	1.92	0.52
1:A:172:LYS:O	1:A:291:ASN:CB	2.53	0.52
1:B:80:VAL:HB	1:B:89:LEU:HG	1.91	0.52
1:B:37:PHE:HA	1:B:334:ASN:O	2.09	0.52
1:B:244:TYR:HB3	1:B:245:PRO:HD2	1.91	0.52
1:A:116:ARG:CD	5:A:822:HOH:O	2.43	0.52
1:B:261:HIS:O	1:B:262:LEU:O	2.28	0.52
1:A:262:LEU:CD1	1:A:266:LYS:HB2	2.40	0.52
1:A:329:THR:HB	1:B:196:PRO:CB	2.40	0.52
1:A:197:PRO:HG2	1:B:330:GLY:O	2.09	0.52
1:A:181:SER:N	3:A:601:AMP:O2P	2.43	0.52
1:B:348:VAL:HG12	1:B:350:LEU:HG	1.92	0.52
1:B:293:MET:HB2	1:B:314:GLN:HB3	1.92	0.52
1:A:74:ALA:HB3	1:A:93:GLU:O	2.09	0.52
1:B:129:GLU:HB2	1:B:185:SER:CB	2.39	0.52
1:A:170:VAL:HB	1:A:294:ILE:CD1	2.35	0.52
1:B:141:ASP:HA	5:B:827:HOH:O	2.08	0.52
1:A:24:GLU:O	1:A:37:PHE:HB2	2.10	0.52
1:A:121:PHE:HE2	1:A:164:SER:O	1.93	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:210:PHE:O	1:A:214:GLY:HA2	2.10	0.52
1:A:344:VAL:HG13	5:A:813:HOH:O	2.09	0.52
1:B:50:SER:HB2	1:B:288:PRO:HB3	1.91	0.52
1:A:331:CYS:HA	5:A:633:HOH:O	2.08	0.52
1:B:290:TYR:CB	1:B:317:PRO:HA	2.39	0.52
1:A:24:GLU:HG3	1:B:118:ILE:O	2.10	0.52
1:A:209:TYR:CD1	1:A:217:CYS:HB3	2.45	0.52
1:A:274:LEU:O	1:A:277:MET:HB2	2.10	0.52
1:A:155:ARG:NH1	1:A:158:GLN:OE1	2.40	0.52
1:A:291:ASN:HB3	1:A:293:MET:SD	2.50	0.52
1:B:32:ASN:ND2	1:B:205:GLY:CA	2.73	0.52
1:B:256:SER:O	1:B:311:TRP:HD1	1.93	0.52
1:A:45:PRO:HG3	1:A:336:VAL:HG13	1.91	0.52
1:B:342:ALA:O	1:B:346:ARG:HG3	2.10	0.52
1:B:95:LEU:HB2	3:B:602:AMP:C2	2.45	0.52
1:B:103:LEU:HD13	1:B:119:VAL:HB	1.92	0.52
1:A:344:VAL:HG13	5:A:811:HOH:O	2.09	0.52
1:A:162:HIS:C	1:A:164:SER:H	2.13	0.52
1:B:103:LEU:O	1:B:106:GLN:HB2	2.09	0.52
1:B:292:TYR:CE1	1:B:313:LEU:HD11	2.45	0.51
1:A:334:ASN:ND2	1:A:334:ASN:C	2.63	0.51
1:B:36:ILE:O	1:B:333:ILE:HA	2.10	0.51
1:B:155:ARG:O	1:B:159:ILE:HG13	2.09	0.51
1:A:184:HIS:HB2	5:A:630:HOH:O	2.10	0.51
1:A:120:GLY:HA2	1:B:25:LEU:HD23	1.91	0.51
1:A:181:SER:OG	3:A:601:AMP:H5'1	2.09	0.51
1:B:292:TYR:O	1:B:293:MET:HE2	2.10	0.51
1:A:228:ILE:HG12	1:A:342:ALA:HA	1.92	0.51
1:A:212:GLU:HG3	1:A:213:THR:CG2	2.40	0.51
1:B:239:PRO:HG2	1:B:242:ALA:HB2	1.92	0.51
1:B:94:ASN:O	1:B:97:PRO:HD3	2.10	0.51
1:A:306:LEU:HB2	1:A:307:PRO:HD3	1.91	0.51
1:A:285:LEU:HD13	1:A:319:LEU:HD21	1.91	0.51
1:A:254:ASP:OD2	5:A:860:HOH:O	2.18	0.51
1:A:327:ILE:HG21	1:B:293:MET:HE3	1.92	0.51
1:A:145:ILE:O	1:A:148:ILE:N	2.44	0.51
1:B:250:ILE:HD12	1:B:315:ILE:HD11	1.91	0.51
1:A:342:ALA:O	1:A:346:ARG:CG	2.58	0.51
1:A:182:MET:N	3:A:601:AMP:O2P	2.42	0.51
1:B:24:GLU:O	1:B:25:LEU:HD22	2.10	0.51
1:B:27:LYS:HD2	1:B:34:TRP:CD1	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:332:TYR:N	1:B:332:TYR:HD2	2.05	0.51
1:A:81:PRO:HD3	1:A:88:LYS:HG3	1.92	0.51
1:A:277:MET:HA	1:A:277:MET:HE2	1.91	0.51
1:A:145:ILE:HA	1:A:148:ILE:HD12	1.93	0.51
1:A:276:LEU:HG	1:A:277:MET:CE	2.40	0.51
1:A:301:VAL:HG13	1:A:301:VAL:O	2.11	0.51
1:B:81:PRO:HB2	1:B:84:ASP:CB	2.40	0.51
1:A:256:SER:HA	5:A:704:HOH:O	2.09	0.51
1:A:283:LYS:HG2	1:A:348:VAL:HG13	1.92	0.51
1:A:137:LEU:HD23	1:A:278:LEU:HD11	1.91	0.51
1:A:129:GLU:OE1	1:A:186:HIS:C	2.48	0.51
1:A:76:GLU:OE1	1:A:79:ARG:HB3	2.09	0.51
1:B:279:GLN:HG2	5:B:648:HOH:O	2.10	0.51
1:B:33:ARG:NH1	1:B:243:THR:OG1	2.43	0.51
1:B:239:PRO:CD	1:B:242:ALA:HB2	2.40	0.51
1:A:28:ASP:C	1:A:30:VAL:H	2.14	0.51
1:A:170:VAL:HG11	1:A:294:ILE:HD12	1.92	0.51
1:B:46:THR:HG23	1:B:47:ASP:N	2.19	0.51
1:A:102:ASN:C	1:A:104:GLU:H	2.14	0.51
1:B:277:MET:HE2	1:B:277:MET:HA	1.93	0.51
1:A:74:ALA:HB3	1:A:93:GLU:O	2.11	0.51
1:A:226:PHE:CE2	1:A:338:PRO:HG2	2.44	0.51
1:B:133:HIS:HA	1:B:184:HIS:ND1	2.24	0.51
1:A:137:LEU:HA	1:A:140:ILE:HD12	1.93	0.51
1:B:38:SER:O	1:B:335:PRO:HA	2.10	0.51
1:A:198:THR:HG23	1:B:330:GLY:CA	2.41	0.51
1:B:166:ASN:ND2	1:B:300:LYS:HD2	2.26	0.51
1:B:218:LEU:HD12	1:B:310:HIS:O	2.10	0.51
1:B:25:LEU:HD22	1:B:36:ILE:HG12	1.92	0.51
1:A:48:PHE:CE2	1:A:336:VAL:HG22	2.45	0.51
1:A:65:PHE:O	1:A:87:TRP:CH2	2.59	0.51
1:A:165:ILE:C	1:A:166:ASN:HD22	2.13	0.51
1:B:70:GLU:CD	1:B:70:GLU:N	2.62	0.51
1:B:269:ASP:O	1:B:270:LEU:C	2.48	0.51
1:B:209:TYR:O	1:B:212:GLU:HB2	2.11	0.51
1:B:231:SER:O	1:B:233:HIS:N	2.44	0.51
1:B:165:ILE:HG22	1:B:299:LEU:CD1	2.38	0.51
1:A:99:LEU:HD21	1:B:36:ILE:HD13	1.93	0.51
1:A:28:ASP:OD1	1:A:30:VAL:HG23	2.11	0.51
1:A:51:LYS:NZ	1:A:320:SER:HA	2.25	0.51
1:A:46:THR:HB	1:A:344:VAL:HG21	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:88:LYS:HD3	5:B:800:HOH:O	2.11	0.51
1:B:105:THR:OG1	5:B:699:HOH:O	2.19	0.51
1:A:116:ARG:HH22	1:B:224:LYS:HD3	1.76	0.51
1:B:177:SER:O	1:B:318:GLN:NE2	2.44	0.51
1:A:216:CYS:O	1:A:220:GLU:HG2	2.11	0.51
1:A:133:HIS:CE1	1:A:184:HIS:HB2	2.46	0.51
1:A:176:ALA:HA	1:A:180:ALA:O	2.11	0.51
1:A:220:GLU:O	1:A:224:LYS:HG2	2.11	0.51
1:A:117:THR:HA	1:B:34:TRP:HZ3	1.76	0.51
1:A:246:PHE:CE2	1:A:341:VAL:HG22	2.45	0.51
1:A:256:SER:HB3	5:A:873:HOH:O	2.11	0.51
1:A:307:PRO:HA	5:A:658:HOH:O	2.10	0.51
1:A:350:LEU:N	5:A:815:HOH:O	2.33	0.51
1:A:224:LYS:HA	1:A:224:LYS:HE2	1.91	0.51
1:A:83:HIS:O	1:A:84:ASP:HB2	2.10	0.51
1:B:227:VAL:HG21	5:B:754:HOH:O	2.11	0.51
1:A:137:LEU:HB2	1:A:172:LYS:HE2	1.92	0.50
1:B:169:GLN:NE2	1:B:293:MET:HB3	2.26	0.50
1:A:156:ILE:HG13	1:A:189:MET:HE3	1.93	0.50
1:B:184:HIS:O	1:B:186:HIS:NE2	2.44	0.50
1:A:66:CYS:SG	1:A:133:HIS:HB2	2.51	0.50
1:B:188:GLN:NE2	3:B:602:AMP:O1P	2.44	0.50
1:B:245:PRO:HD2	5:B:632:HOH:O	2.11	0.50
1:A:75:PRO:HG3	5:A:777:HOH:O	2.11	0.50
1:B:209:TYR:HE1	1:B:215:LYS:HB2	1.76	0.50
1:A:217:CYS:SG	5:A:769:HOH:O	2.60	0.50
1:A:165:ILE:HG21	1:A:191:ALA:HB1	1.92	0.50
1:A:78:PHE:HB3	5:A:785:HOH:O	2.10	0.50
1:A:325:PHE:CE1	1:B:192:LEU:HD21	2.45	0.50
1:A:186:HIS:CD2	3:A:601:AMP:P	3.04	0.50
1:B:233:HIS:CG	1:B:266:LYS:HG2	2.47	0.50
1:B:101:ARG:CD	5:B:698:HOH:O	2.58	0.50
1:A:22:SER:O	1:A:22:SER:OG	2.29	0.50
1:A:266:LYS:HE3	5:A:804:HOH:O	2.10	0.50
1:B:196:PRO:HG2	1:B:199:VAL:HG23	1.93	0.50
1:B:48:PHE:HB2	1:B:246:PHE:CE1	2.46	0.50
1:A:90:ARG:CZ	5:A:708:HOH:O	2.58	0.50
1:A:262:LEU:HD11	1:A:266:LYS:CB	2.42	0.50
1:A:266:LYS:O	1:A:267:ALA:C	2.48	0.50
1:A:160:ALA:O	1:A:162:HIS:N	2.44	0.50
1:A:141:ASP:HB2	1:A:142:PRO:CD	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:87:TRP:CE2	1:B:90:ARG:HD3	2.46	0.50
1:A:184:HIS:HB3	1:A:186:HIS:CD2	2.47	0.50
1:B:80:VAL:HB	1:B:89:LEU:HG	1.93	0.50
1:B:276:LEU:HD13	5:B:769:HOH:O	2.11	0.50
1:A:123:PHE:HB2	1:A:191:ALA:HB3	1.93	0.50
1:A:89:LEU:HD12	1:A:89:LEU:C	2.32	0.50
1:B:228:ILE:HG13	1:B:237:VAL:HA	1.93	0.50
1:B:176:ALA:HA	1:B:180:ALA:O	2.11	0.50
1:A:78:PHE:HE1	1:A:154:LYS:HD3	1.75	0.50
1:A:158:GLN:HG3	5:A:702:HOH:O	2.10	0.50
1:B:148:ILE:O	1:B:151:ALA:HB3	2.11	0.50
1:A:44:ARG:HB3	1:A:47:ASP:OD1	2.11	0.50
1:A:128:ILE:HA	1:A:186:HIS:HB3	1.93	0.50
1:B:175:GLY:O	1:B:180:ALA:HB3	2.10	0.50
1:A:70:GLU:H	1:A:70:GLU:CD	2.15	0.50
1:B:49:LYS:CD	1:B:286:ASN:HD21	2.12	0.50
1:B:25:LEU:HA	1:B:35:VAL:O	2.11	0.50
1:A:281:ILE:CG2	1:A:285:LEU:HD12	2.36	0.50
1:A:292:TYR:HA	1:A:314:GLN:O	2.10	0.50
1:B:252:PRO:HD2	1:B:311:TRP:O	2.12	0.50
1:B:146:GLY:O	1:B:150:ILE:HG12	2.11	0.50
1:B:118:ILE:HG13	1:B:118:ILE:O	2.12	0.50
1:B:49:LYS:HA	1:B:285:LEU:HD23	1.93	0.50
1:A:28:ASP:HB2	5:A:623:HOH:O	2.12	0.50
1:A:170:VAL:CG1	1:A:294:ILE:HD12	2.42	0.50
1:A:125:ASP:OD2	1:A:155:ARG:NH2	2.42	0.50
1:B:30:VAL:HG12	4:B:611:EDO:H11	1.93	0.50
1:A:324:GLY:H	1:B:173:ASN:ND2	2.09	0.50
1:B:216:CYS:SG	1:B:255:HIS:HE1	2.33	0.50
1:B:177:SER:C	1:B:318:GLN:HE22	2.15	0.50
1:A:138:SER:HB3	1:A:278:LEU:HB3	1.92	0.50
1:B:98:ALA:O	1:B:99:LEU:HD23	2.11	0.50
1:B:66:CYS:SG	1:B:133:HIS:HB2	2.51	0.50
1:B:104:GLU:OE2	1:B:162:HIS:ND1	2.44	0.50
1:B:87:TRP:CH2	1:B:131:PRO:HA	2.46	0.50
1:B:188:GLN:NE2	3:B:602:AMP:H5'2	2.26	0.50
1:A:242:ALA:O	1:A:334:ASN:ND2	2.45	0.50
1:A:300:LYS:NZ	5:A:730:HOH:O	2.44	0.50
1:B:101:ARG:NH2	5:B:699:HOH:O	2.23	0.50
1:B:207:LYS:HB2	1:B:308:TYR:CZ	2.47	0.50
1:B:80:VAL:HB	1:B:89:LEU:HG	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:218:LEU:HB2	1:B:310:HIS:ND1	2.26	0.50
1:A:171:PHE:HA	1:A:292:TYR:O	2.12	0.50
1:A:103:LEU:O	1:A:106:GLN:HG2	2.12	0.50
1:A:191:ALA:O	1:A:192:LEU:HD23	2.12	0.50
1:B:25:LEU:HA	1:B:35:VAL:O	2.12	0.49
1:B:81:PRO:HD3	1:B:88:LYS:HG3	1.94	0.49
1:B:173:ASN:CG	1:B:291:ASN:ND2	2.65	0.49
1:B:188:GLN:NE2	3:B:602:AMP:H5'2	2.27	0.49
1:A:149:LEU:CD1	1:A:270:LEU:HD23	2.42	0.49
1:A:210:PHE:HB2	1:A:308:TYR:HB3	1.93	0.49
5:A:738:HOH:O	1:B:117:THR:HG22	2.11	0.49
1:A:232:SER:HB2	1:A:269:ASP:OD1	2.12	0.49
1:A:279:GLN:HG2	1:A:350:LEU:CD1	2.40	0.49
1:B:213:THR:HB	1:B:215:LYS:CE	2.42	0.49
1:A:244:TYR:O	4:A:607:EDO:H11	2.12	0.49
1:B:242:ALA:CB	4:B:610:EDO:H11	2.43	0.49
1:B:270:LEU:O	1:B:270:LEU:HD12	2.11	0.49
1:A:155:ARG:HD2	1:A:158:GLN:HB2	1.93	0.49
1:B:257:SER:O	1:B:297:SER:HB2	2.11	0.49
1:B:318:GLN:HA	4:B:612:EDO:H11	1.94	0.49
1:B:132:VAL:HG12	1:B:133:HIS:N	2.27	0.49
1:A:23:PRO:C	1:A:24:GLU:HG3	2.32	0.49
1:A:242:ALA:CB	4:A:607:EDO:H11	2.42	0.49
1:A:35:VAL:HG22	1:A:36:ILE:N	2.27	0.49
1:B:234:PHE:HE2	1:B:252:PRO:HD3	1.78	0.49
1:A:319:LEU:O	1:A:320:SER:C	2.51	0.49
1:A:127:VAL:N	1:A:187:SER:O	2.44	0.49
1:A:175:GLY:HA3	1:A:289:PRO:HB3	1.95	0.49
1:B:27:LYS:HA	1:B:33:ARG:O	2.12	0.49
1:A:31:THR:HB	5:A:770:HOH:O	2.12	0.49
1:B:21:GLN:NE2	5:B:764:HOH:O	2.44	0.49
1:B:222:LYS:O	5:B:754:HOH:O	2.19	0.49
1:A:141:ASP:O	1:A:144:GLY:N	2.45	0.49
1:A:182:MET:HB2	1:A:186:HIS:CE1	2.47	0.49
1:A:81:PRO:HD3	1:A:88:LYS:HG3	1.93	0.49
1:A:135:ILE:HG23	1:A:139:ASP:HB2	1.93	0.49
1:B:295:HIS:O	1:B:311:TRP:HB2	2.13	0.49
1:B:218:LEU:HD12	1:B:310:HIS:CB	2.36	0.49
1:B:310:HIS:HD2	1:B:311:TRP:H	1.59	0.49
1:B:48:PHE:O	1:B:49:LYS:HG3	2.12	0.49
1:A:322:VAL:HB	1:A:326:GLU:OE2	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:182:MET:HA	1:B:182:MET:HE2	1.95	0.49
1:A:226:PHE:CE2	1:A:339:GLU:HG3	2.46	0.49
1:A:127:VAL:O	1:A:186:HIS:HB2	2.12	0.49
1:A:91:VAL:HA	1:A:126:VAL:O	2.12	0.49
1:B:117:THR:HG22	1:B:118:ILE:N	2.28	0.49
1:B:227:VAL:O	1:B:346:ARG:CZ	2.60	0.49
3:A:601:AMP:H2'	5:A:674:HOH:O	2.13	0.49
1:A:76:GLU:OE1	1:A:79:ARG:HB3	2.12	0.49
1:B:37:PHE:HE2	1:B:241:ALA:HA	1.78	0.49
1:B:123:PHE:HB2	1:B:191:ALA:HB3	1.94	0.49
1:B:140:ILE:CG2	1:B:141:ASP:N	2.75	0.49
1:B:140:ILE:HG22	1:B:141:ASP:N	2.27	0.49
1:B:153:LYS:HE3	5:B:737:HOH:O	2.12	0.49
1:A:285:LEU:HD13	1:A:319:LEU:HD11	1.95	0.49
1:B:326:GLU:C	1:B:328:GLY:N	2.65	0.49
1:A:329:THR:HG22	1:B:169:GLN:OE1	2.12	0.49
1:B:231:SER:HB2	1:B:269:ASP:OD1	2.13	0.49
1:A:51:LYS:HE2	1:A:319:LEU:O	2.13	0.49
1:A:265:VAL:N	5:A:805:HOH:O	2.46	0.49
1:A:71:GLN:OE1	1:A:71:GLN:HA	2.12	0.49
1:A:256:SER:O	1:A:310:HIS:HD2	1.96	0.49
1:A:278:LEU:HD22	1:A:290:TYR:CZ	2.47	0.49
1:A:133:HIS:HB3	5:A:761:HOH:O	2.11	0.49
1:A:258:HIS:CE1	1:A:297:SER:HB3	2.48	0.49
1:A:324:GLY:HA3	1:B:171:PHE:HB2	1.95	0.49
1:B:127:VAL:O	1:B:187:SER:N	2.44	0.49
1:A:50:SER:CB	1:A:288:PRO:HB3	2.41	0.49
1:A:45:PRO:HG2	1:A:340:ASP:OD2	2.12	0.49
1:B:248:ILE:HD12	1:B:281:ILE:HD11	1.94	0.49
1:A:48:PHE:O	1:A:49:LYS:HD3	2.13	0.49
1:B:269:ASP:O	1:B:271:GLY:N	2.46	0.49
1:A:106:GLN:O	1:A:107:SER:HB2	2.13	0.49
1:B:233:HIS:NE2	5:B:669:HOH:O	2.34	0.49
1:B:64:PRO:HD3	5:B:793:HOH:O	2.13	0.49
1:B:298:PRO:HD2	1:B:301:VAL:HB	1.94	0.49
1:A:228:ILE:HD11	1:A:238:ALA:HB2	1.94	0.49
1:B:66:CYS:O	1:B:69:ARG:HB2	2.13	0.49
1:B:119:VAL:O	1:B:121:PHE:N	2.38	0.49
1:A:95:LEU:HD23	1:A:96:TYR:CE1	2.48	0.49
1:B:185:SER:HB3	5:B:692:HOH:O	2.12	0.49
1:B:27:LYS:HG3	1:B:33:ARG:C	2.33	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:27:LYS:HG3	1:B:33:ARG:N	2.28	0.49
1:A:226:PHE:C	1:A:237:VAL:HB	2.33	0.49
1:B:26:ARG:HH12	1:B:338:PRO:CG	2.25	0.49
1:B:23:PRO:HA	1:B:37:PHE:O	2.12	0.49
1:A:329:THR:HB	1:B:196:PRO:CB	2.42	0.49
1:B:100:SER:HB3	1:B:103:LEU:HD12	1.95	0.49
1:B:87:TRP:CE2	1:B:90:ARG:HD2	2.48	0.49
1:B:101:ARG:HA	1:B:121:PHE:CD1	2.48	0.49
1:B:265:VAL:CG1	5:B:652:HOH:O	2.58	0.49
1:B:326:GLU:HA	1:B:331:CYS:O	2.13	0.49
1:A:318:GLN:HG2	4:A:609:EDO:O1	2.13	0.49
1:A:198:THR:HG23	1:B:329:THR:C	2.33	0.49
1:A:213:THR:HB	1:A:215:LYS:NZ	2.28	0.49
1:A:324:GLY:HA2	1:B:293:MET:HE1	1.95	0.49
1:A:228:ILE:HG12	1:A:342:ALA:HA	1.94	0.49
1:A:87:TRP:CH2	1:A:131:PRO:HA	2.48	0.49
1:A:106:GLN:O	1:A:107:SER:CB	2.60	0.49
1:A:329:THR:O	1:B:197:PRO:HD2	2.13	0.49
1:B:137:LEU:HD23	1:B:137:LEU:C	2.33	0.49
1:B:265:VAL:HG13	5:B:653:HOH:O	2.13	0.49
1:B:332:TYR:O	1:B:333:ILE:HG13	2.13	0.49
1:B:226:PHE:HD2	1:B:338:PRO:HB2	1.77	0.49
1:A:89:LEU:C	1:A:89:LEU:HD12	2.32	0.49
1:A:29:PRO:O	1:A:205:GLY:HA3	2.13	0.48
1:B:50:SER:C	1:B:286:ASN:HD22	2.17	0.48
1:A:78:PHE:N	1:A:78:PHE:CD2	2.81	0.48
1:A:132:VAL:HG11	1:A:135:ILE:CD1	2.43	0.48
1:A:132:VAL:HB	1:A:135:ILE:HD12	1.94	0.48
1:A:328:GLY:HA3	1:B:293:MET:HG2	1.95	0.48
1:A:77:LEU:O	1:A:78:PHE:HB3	2.13	0.48
1:B:25:LEU:HD13	1:B:36:ILE:HA	1.94	0.48
1:A:280:LYS:HE2	1:A:350:LEU:HD12	1.95	0.48
1:B:137:LEU:HD22	1:B:172:LYS:HD2	1.94	0.48
1:A:69:ARG:O	1:A:72:GLU:HB2	2.12	0.48
1:A:199:VAL:O	1:A:203:LEU:HG	2.13	0.48
1:B:30:VAL:O	1:B:202:ARG:HB2	2.13	0.48
1:B:26:ARG:NH1	1:B:338:PRO:CG	2.76	0.48
1:A:329:THR:C	1:B:198:THR:HG23	2.34	0.48
1:B:262:LEU:HD12	1:B:266:LYS:CB	2.43	0.48
1:B:180:ALA:HA	3:B:602:AMP:O2P	2.13	0.48
1:B:239:PRO:HG3	1:B:249:TRP:CG	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:234:PHE:HB3	1:A:273:LEU:HD23	1.94	0.48
1:B:307:PRO:HG2	5:B:783:HOH:O	2.12	0.48
1:B:143:VAL:HG22	1:B:268:VAL:HG11	1.96	0.48
1:A:26:ARG:HD2	1:A:37:PHE:CE2	2.48	0.48
1:A:324:GLY:H	1:B:173:ASN:HD21	1.61	0.48
1:A:175:GLY:HA3	1:A:289:PRO:HB3	1.94	0.48
1:A:332:TYR:CD2	1:A:332:TYR:N	2.82	0.48
1:B:276:LEU:CG	1:B:280:LYS:HE3	2.43	0.48
1:B:266:LYS:O	1:B:270:LEU:N	2.42	0.48
1:B:129:GLU:OE2	1:B:137:LEU:HD12	2.14	0.48
1:B:28:ASP:OD1	1:B:30:VAL:HG23	2.13	0.48
1:A:133:HIS:CE1	5:A:630:HOH:O	2.58	0.48
1:A:197:PRO:HD3	5:B:785:HOH:O	2.12	0.48
1:B:31:THR:OG1	1:B:33:ARG:HG2	2.13	0.48
1:A:166:ASN:HB3	1:A:195:VAL:HG22	1.94	0.48
1:A:285:LEU:O	1:A:286:ASN:HB2	2.14	0.48
1:A:222:LYS:HE3	5:A:799:HOH:O	2.12	0.48
1:A:143:VAL:HA	1:A:268:VAL:HG22	1.93	0.48
1:B:121:PHE:CD1	1:B:122:GLY:N	2.82	0.48
1:A:285:LEU:O	1:A:286:ASN:HB2	2.13	0.48
1:A:248:ILE:HB	1:A:315:ILE:HB	1.95	0.48
1:A:307:PRO:CA	5:A:658:HOH:O	2.61	0.48
1:A:349:SER:HA	5:A:815:HOH:O	2.12	0.48
1:B:50:SER:HB3	1:B:286:ASN:O	2.13	0.48
1:A:254:ASP:O	1:A:255:HIS:C	2.52	0.48
1:A:140:ILE:HG22	1:A:141:ASP:N	2.28	0.48
1:B:258:HIS:HD2	1:B:261:HIS:CE1	2.31	0.48
1:A:227:VAL:HG13	1:A:235:VAL:CG2	2.44	0.48
1:B:106:GLN:O	1:B:107:SER:CB	2.57	0.48
1:A:67:ILE:HG13	1:A:87:TRP:NE1	2.28	0.48
1:B:182:MET:SD	3:B:602:AMP:C8	3.06	0.48
1:B:63:CYS:SG	1:B:65:PHE:HB2	2.53	0.48
1:A:262:LEU:HD11	1:A:266:LYS:HB3	1.96	0.48
1:A:182:MET:HB2	1:A:186:HIS:NE2	2.28	0.48
1:A:236:SER:HA	1:A:249:TRP:O	2.14	0.48
1:B:25:LEU:CD1	1:B:36:ILE:HG12	2.38	0.48
1:A:26:ARG:HB2	1:A:37:PHE:HE2	1.78	0.48
1:B:87:TRP:CE2	1:B:90:ARG:HD2	2.48	0.48
1:A:292:TYR:HA	1:A:314:GLN:O	2.14	0.48
1:A:306:LEU:N	1:A:307:PRO:HD3	2.29	0.48
1:B:259:PHE:O	1:B:262:LEU:HD22	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:207:LYS:O	1:A:208:ASP:C	2.52	0.48
1:B:311:TRP:HZ2	5:B:682:HOH:O	1.96	0.48
1:A:171:PHE:CD2	1:A:171:PHE:N	2.82	0.48
1:A:161:GLN:NE2	5:A:851:HOH:O	2.46	0.48
1:A:329:THR:HB	1:B:196:PRO:HB2	1.95	0.48
1:B:87:TRP:CH2	1:B:131:PRO:HA	2.48	0.48
1:A:306:LEU:O	1:A:308:TYR:N	2.47	0.48
1:A:168:ILE:HG13	1:A:299:LEU:HD11	1.94	0.48
1:A:63:CYS:SG	1:A:65:PHE:HB2	2.54	0.48
1:B:297:SER:HB3	1:B:309:THR:HG21	1.96	0.48
1:A:106:GLN:OE1	1:A:106:GLN:HA	2.13	0.48
1:A:100:SER:O	1:A:121:PHE:HA	2.13	0.48
1:B:100:SER:CB	1:B:103:LEU:HG	2.44	0.48
1:B:292:TYR:C	1:B:293:MET:SD	2.92	0.48
1:B:292:TYR:HA	1:B:314:GLN:O	2.13	0.48
1:A:255:HIS:HA	1:A:310:HIS:ND1	2.29	0.48
1:B:285:LEU:C	1:B:288:PRO:HD3	2.34	0.48
1:A:25:LEU:HB2	1:B:118:ILE:HG13	1.96	0.48
1:B:206:THR:HG22	1:B:217:CYS:SG	2.53	0.48
1:A:67:ILE:HG22	5:A:843:HOH:O	2.13	0.48
1:A:30:VAL:HG13	1:A:202:ARG:HD3	1.95	0.48
1:A:329:THR:HA	1:B:198:THR:OG1	2.14	0.48
1:A:258:HIS:HB2	1:A:260:HIS:CE1	2.49	0.48
1:B:137:LEU:O	1:B:140:ILE:HB	2.14	0.48
1:A:26:ARG:HD2	1:A:37:PHE:HE2	1.78	0.48
1:B:338:PRO:HA	4:B:610:EDO:H22	1.94	0.48
1:A:79:ARG:HH22	1:A:85:PRO:HA	1.78	0.48
1:A:87:TRP:CH2	1:A:131:PRO:HA	2.47	0.48
1:A:329:THR:C	1:A:331:CYS:H	2.17	0.48
1:B:132:VAL:HG12	1:B:135:ILE:H	1.78	0.48
1:B:89:LEU:HD22	1:B:148:ILE:HA	1.96	0.48
1:B:33:ARG:HH22	1:B:243:THR:HG1	1.58	0.48
1:A:285:LEU:HB2	1:A:288:PRO:CD	2.43	0.48
1:B:203:LEU:HD13	1:B:305:GLN:HE21	1.78	0.48
1:A:63:CYS:HB2	1:A:64:PRO:CD	2.43	0.48
1:A:29:PRO:HB3	1:A:205:GLY:O	2.14	0.48
1:A:234:PHE:CE1	1:A:270:LEU:HB2	2.49	0.48
1:B:310:HIS:CD2	1:B:311:TRP:N	2.82	0.48
1:B:239:PRO:CG	1:B:242:ALA:HB2	2.44	0.48
1:A:186:HIS:CD2	3:A:601:AMP:P	3.06	0.48
1:A:129:GLU:OE2	1:A:185:SER:OG	2.32	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:325:PHE:HE1	1:B:192:LEU:HD11	1.79	0.48
1:B:262:LEU:HD12	1:B:266:LYS:HB2	1.95	0.48
1:B:167:TYR:HD2	1:B:298:PRO:HA	1.79	0.48
1:A:123:PHE:HB2	1:A:191:ALA:HB3	1.96	0.48
1:B:78:PHE:HD2	1:B:158:GLN:HE22	1.61	0.48
1:A:80:VAL:HB	1:A:89:LEU:HG	1.95	0.48
1:B:220:GLU:HB3	1:B:223:SER:OG	2.14	0.48
1:A:127:VAL:HG21	1:A:152:TYR:HE1	1.77	0.48
1:A:26:ARG:HG2	1:B:117:THR:OG1	2.13	0.48
1:A:24:GLU:HA	1:B:120:GLY:N	2.29	0.48
1:B:209:TYR:CE2	1:B:213:THR:HG21	2.48	0.48
1:A:90:ARG:HB2	1:A:128:ILE:CD1	2.41	0.48
1:B:273:LEU:HD12	1:B:277:MET:CE	2.40	0.48
1:A:132:VAL:CG1	1:A:135:ILE:HG13	2.44	0.48
1:A:210:PHE:HB2	1:A:308:TYR:HB3	1.95	0.48
1:A:106:GLN:O	1:A:107:SER:HB2	2.14	0.48
1:B:64:PRO:HD3	5:B:795:HOH:O	2.14	0.48
1:A:50:SER:HB2	1:A:288:PRO:CB	2.39	0.48
1:A:292:TYR:O	1:A:293:MET:HG3	2.13	0.48
1:B:48:PHE:CZ	1:B:336:VAL:HG22	2.49	0.48
1:B:150:ILE:HG22	1:B:150:ILE:O	2.14	0.48
1:A:150:ILE:HB	5:A:663:HOH:O	2.13	0.48
1:B:123:PHE:HB2	1:B:191:ALA:HB3	1.95	0.47
1:A:220:GLU:HB3	1:A:224:LYS:HG2	1.96	0.47
1:A:244:TYR:CD2	1:A:316:VAL:HG21	2.49	0.47
1:B:129:GLU:OE2	1:B:172:LYS:NZ	2.47	0.47
1:A:170:VAL:HG13	1:A:189:MET:HG2	1.95	0.47
1:B:29:PRO:HG3	5:B:657:HOH:O	2.14	0.47
1:A:94:ASN:O	1:A:97:PRO:HD3	2.14	0.47
1:A:301:VAL:CG2	1:A:305:GLN:HB2	2.41	0.47
1:A:49:LYS:HD2	1:A:286:ASN:HD21	1.77	0.47
1:A:117:THR:HG23	1:B:26:ARG:HG3	1.96	0.47
1:B:46:THR:HB	1:B:344:VAL:CG2	2.44	0.47
1:B:247:GLU:HA	1:B:315:ILE:O	2.14	0.47
1:B:175:GLY:C	1:B:180:ALA:HB3	2.34	0.47
1:A:235:VAL:HG22	1:A:236:SER:O	2.14	0.47
1:B:93:GLU:HA	1:B:125:ASP:OD1	2.14	0.47
1:A:245:PRO:O	1:A:246:PHE:HB2	2.12	0.47
1:B:172:LYS:O	1:B:292:TYR:N	2.33	0.47
1:A:283:LYS:HD3	1:A:350:LEU:HD23	1.96	0.47
1:A:318:GLN:HE21	4:A:609:EDO:C2	2.27	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:80:VAL:HA	1:A:81:PRO:C	2.34	0.47
1:A:257:SER:HB2	1:A:258:HIS:CE1	2.49	0.47
1:A:245:PRO:O	1:A:246:PHE:HB2	2.13	0.47
1:B:106:GLN:HE21	1:B:119:VAL:HG11	1.78	0.47
1:A:116:ARG:NH2	1:B:224:LYS:HD2	2.29	0.47
1:B:197:PRO:O	1:B:201:SER:OG	2.28	0.47
1:B:289:PRO:HG2	1:B:318:GLN:NE2	2.28	0.47
1:A:23:PRO:HG3	5:B:719:HOH:O	2.14	0.47
1:B:264:ASP:O	1:B:268:VAL:HG23	2.14	0.47
1:B:226:PHE:CE1	1:B:339:GLU:HG3	2.48	0.47
1:B:96:TYR:N	1:B:97:PRO:CD	2.77	0.47
1:B:28:ASP:HB3	1:B:31:THR:OG1	2.14	0.47
1:B:325:PHE:CD2	1:B:333:ILE:HD11	2.48	0.47
1:A:292:TYR:C	1:A:293:MET:HG3	2.33	0.47
1:B:50:SER:HB2	1:B:288:PRO:CA	2.44	0.47
1:B:65:PHE:CD2	1:B:128:ILE:HG12	2.49	0.47
1:A:76:GLU:HB2	1:A:90:ARG:NH2	2.30	0.47
1:A:165:ILE:HG22	1:A:299:LEU:HD11	1.96	0.47
1:A:51:LYS:CE	1:A:320:SER:HA	2.44	0.47
1:B:24:GLU:O	1:B:37:PHE:HB2	2.14	0.47
1:A:129:GLU:OE2	1:A:185:SER:OG	2.32	0.47
1:A:281:ILE:HG23	1:A:285:LEU:HD12	1.96	0.47
1:B:325:PHE:CE1	1:B:329:THR:HG21	2.50	0.47
1:A:154:LYS:HG2	1:A:158:GLN:HE21	1.79	0.47
1:B:94:ASN:ND2	3:B:602:AMP:O3'	2.36	0.47
1:B:101:ARG:HD2	5:B:699:HOH:O	2.15	0.47
1:B:227:VAL:HG23	5:B:758:HOH:O	2.13	0.47
1:A:205:GLY:O	1:A:206:THR:C	2.51	0.47
1:B:263:ASP:OD2	1:B:266:LYS:N	2.40	0.47
1:B:21:GLN:OE1	5:B:776:HOH:O	2.20	0.47
1:A:177:SER:OG	1:A:289:PRO:HG2	2.14	0.47
1:A:199:VAL:HG11	1:A:298:PRO:HG3	1.96	0.47
1:A:297:SER:O	1:A:298:PRO:C	2.53	0.47
1:B:238:ALA:HB1	4:B:610:EDO:H12	1.97	0.47
1:A:271:GLY:O	1:A:272:GLY:C	2.53	0.47
1:A:61:SER:HA	5:A:842:HOH:O	2.15	0.47
1:A:234:PHE:CE1	1:A:270:LEU:HB2	2.50	0.47
1:A:66:CYS:SG	1:A:133:HIS:HB2	2.53	0.47
1:B:257:SER:HA	1:B:309:THR:O	2.14	0.47
1:A:118:ILE:HG23	1:B:34:TRP:CH2	2.50	0.47
1:A:198:THR:HG23	1:B:329:THR:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:137:LEU:CD2	1:B:172:LYS:HD2	2.44	0.47
1:A:64:PRO:HB3	1:A:72:GLU:HB3	1.96	0.47
1:A:143:VAL:HA	1:A:268:VAL:HG22	1.96	0.47
1:B:174:GLN:O	1:B:289:PRO:HA	2.13	0.47
1:A:218:LEU:HB2	1:A:310:HIS:HB3	1.97	0.47
1:A:329:THR:HB	1:B:196:PRO:HB2	1.94	0.47
1:A:45:PRO:C	1:A:47:ASP:H	2.18	0.47
1:B:235:VAL:HG13	1:B:235:VAL:O	2.14	0.47
1:B:318:GLN:CD	1:B:318:GLN:C	2.72	0.47
1:B:133:HIS:HA	1:B:184:HIS:CE1	2.49	0.47
1:B:62:SER:CB	1:B:69:ARG:HH11	2.27	0.47
1:A:77:LEU:HD13	1:A:155:ARG:NE	2.29	0.47
1:B:288:PRO:HD2	5:B:628:HOH:O	2.14	0.47
1:B:234:PHE:CB	1:B:273:LEU:CD2	2.91	0.47
1:A:170:VAL:HA	1:A:188:GLN:O	2.15	0.47
1:A:266:LYS:CE	5:A:804:HOH:O	2.63	0.47
1:B:25:LEU:CD1	1:B:36:ILE:HG12	2.44	0.47
1:A:213:THR:CB	1:A:215:LYS:HE3	2.37	0.47
1:B:209:TYR:CE1	1:B:215:LYS:HB2	2.50	0.47
1:B:335:PRO:O	1:B:336:VAL:HG23	2.15	0.47
1:B:80:VAL:HB	1:B:89:LEU:HG	1.96	0.47
1:B:129:GLU:HB3	1:B:148:ILE:CD1	2.45	0.47
1:A:207:LYS:HB2	1:A:308:TYR:CE2	2.50	0.47
1:B:250:ILE:HB	1:B:313:LEU:HD22	1.96	0.47
1:A:278:LEU:O	1:A:279:GLN:C	2.53	0.47
1:B:288:PRO:O	1:B:289:PRO:C	2.52	0.47
1:A:306:LEU:N	1:A:307:PRO:HD3	2.30	0.47
1:A:106:GLN:O	1:A:107:SER:HB2	2.15	0.47
1:A:254:ASP:CB	5:A:860:HOH:O	2.63	0.47
1:B:164:SER:O	1:B:193:PRO:HA	2.15	0.47
1:B:153:LYS:HG2	1:B:157:ASN:ND2	2.29	0.47
1:A:324:GLY:H	1:B:173:ASN:CG	2.18	0.47
1:A:236:SER:O	1:A:237:VAL:CG1	2.62	0.47
1:B:245:PRO:HB3	1:B:335:PRO:HD2	1.96	0.47
1:A:161:GLN:HB2	5:A:787:HOH:O	2.15	0.47
1:A:30:VAL:CG1	1:A:202:ARG:HG3	2.42	0.47
1:A:337:PHE:HD1	5:A:700:HOH:O	1.97	0.47
1:A:77:LEU:O	1:A:78:PHE:HB3	2.15	0.47
1:A:257:SER:HA	1:A:309:THR:O	2.14	0.47
1:A:37:PHE:CE2	1:A:241:ALA:HA	2.50	0.47
1:A:146:GLY:HA2	1:A:267:ALA:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:228:ILE:HA	1:B:346:ARG:CG	2.45	0.47
1:A:184:HIS:O	1:A:185:SER:C	2.52	0.47
1:A:123:PHE:HB2	1:A:191:ALA:CB	2.41	0.47
1:A:259:PHE:CD2	1:A:260:HIS:N	2.83	0.47
1:A:235:VAL:O	1:A:236:SER:C	2.53	0.47
1:A:254:ASP:HB2	5:A:687:HOH:O	2.15	0.47
1:B:81:PRO:HB2	1:B:84:ASP:CB	2.44	0.47
1:A:284:GLN:O	1:A:284:GLN:HG3	2.14	0.47
1:A:259:PHE:O	1:A:262:LEU:HD22	2.15	0.47
1:B:129:GLU:OE1	1:B:172:LYS:NZ	2.44	0.47
1:A:76:GLU:OE1	1:A:79:ARG:HB3	2.15	0.47
1:A:197:PRO:CG	1:B:33:ARG:HB2	2.45	0.47
1:A:100:SER:HB3	1:A:103:LEU:CD1	2.45	0.47
1:A:200:SER:HB2	5:A:791:HOH:O	2.15	0.47
1:B:99:LEU:HD22	1:B:121:PHE:O	2.15	0.47
1:B:50:SER:CB	1:B:288:PRO:HB3	2.45	0.47
1:A:162:HIS:O	1:A:164:SER:N	2.47	0.46
1:A:173:ASN:HD22	1:A:188:GLN:HE21	1.62	0.46
1:A:165:ILE:HG23	1:A:191:ALA:HB1	1.97	0.46
1:A:259:PHE:O	1:A:261:HIS:N	2.49	0.46
1:B:263:ASP:OD1	5:B:783:HOH:O	2.20	0.46
1:A:171:PHE:CZ	1:A:188:GLN:HB2	2.50	0.46
1:A:301:VAL:HG22	1:A:305:GLN:HB2	1.97	0.46
1:A:326:GLU:CG	1:A:332:TYR:HA	2.45	0.46
1:B:33:ARG:HH22	1:B:243:THR:CG2	2.28	0.46
1:B:25:LEU:CD1	1:B:36:ILE:HG12	2.41	0.46
1:A:118:ILE:O	1:B:24:GLU:HG3	2.15	0.46
1:A:79:ARG:HD2	1:A:83:HIS:HA	1.97	0.46
1:B:313:LEU:HD23	1:B:313:LEU:C	2.35	0.46
1:B:128:ILE:HG23	1:B:184:HIS:CD2	2.50	0.46
1:B:150:ILE:O	1:B:153:LYS:HB3	2.15	0.46
1:A:117:THR:HG23	1:B:24:GLU:HG3	1.96	0.46
1:A:305:GLN:HA	1:A:308:TYR:OH	2.15	0.46
1:A:226:PHE:CE2	1:A:240:PHE:HD1	2.33	0.46
1:B:234:PHE:HE1	1:B:270:LEU:HB2	1.79	0.46
1:A:175:GLY:H	1:A:180:ALA:CB	2.28	0.46
1:B:177:SER:C	1:B:318:GLN:HE22	2.18	0.46
1:B:258:HIS:CD2	1:B:261:HIS:CE1	3.03	0.46
1:B:93:GLU:HG2	1:B:101:ARG:CZ	2.46	0.46
1:B:347:GLU:O	1:B:349:SER:N	2.48	0.46
1:A:118:ILE:HG13	1:B:25:LEU:HB2	1.95	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:225:HIS:HB3	1:A:237:VAL:HG21	1.96	0.46
1:A:248:ILE:HD12	1:A:281:ILE:CD1	2.39	0.46
1:A:210:PHE:CD2	1:A:308:TYR:HB3	2.51	0.46
1:A:80:VAL:HA	1:A:81:PRO:C	2.34	0.46
1:A:65:PHE:HE2	1:A:182:MET:HG3	1.79	0.46
1:B:175:GLY:HA3	1:B:289:PRO:CB	2.43	0.46
1:A:28:ASP:CB	5:A:623:HOH:O	2.62	0.46
1:A:33:ARG:NH2	1:A:332:TYR:CE2	2.83	0.46
1:B:280:LYS:HA	1:B:348:VAL:HG11	1.97	0.46
1:A:250:ILE:C	1:A:251:ILE:HD12	2.35	0.46
1:B:35:VAL:HG12	1:B:241:ALA:HB1	1.96	0.46
1:B:129:GLU:HB3	1:B:148:ILE:HD13	1.96	0.46
1:B:46:THR:CA	1:B:340:ASP:HB3	2.44	0.46
1:B:46:THR:HA	1:B:340:ASP:HB3	1.97	0.46
1:A:30:VAL:HG11	1:A:312:PHE:CZ	2.49	0.46
1:A:336:VAL:HG12	1:A:341:VAL:HG23	1.96	0.46
1:B:275:LYS:HE3	1:B:279:GLN:OE1	2.15	0.46
1:B:25:LEU:HD22	1:B:36:ILE:CG1	2.34	0.46
1:A:82:ASP:OD1	1:A:83:HIS:ND1	2.46	0.46
1:B:239:PRO:HG3	1:B:249:TRP:CD1	2.50	0.46
1:B:157:ASN:ND2	5:B:642:HOH:O	2.26	0.46
1:B:28:ASP:HB2	5:B:633:HOH:O	2.15	0.46
1:A:44:ARG:HG2	1:A:46:THR:H	1.79	0.46
1:A:132:VAL:HB	1:A:135:ILE:CD1	2.44	0.46
1:B:280:LYS:HG2	1:B:348:VAL:HG11	1.96	0.46
1:B:171:PHE:HZ	1:B:190:MET:HE2	1.81	0.46
1:A:227:VAL:O	1:A:346:ARG:NH2	2.49	0.46
1:B:213:THR:HB	1:B:215:LYS:HE3	1.98	0.46
1:B:169:GLN:HG3	1:B:171:PHE:HD2	1.81	0.46
1:A:67:ILE:HD11	1:A:85:PRO:O	2.15	0.46
1:A:347:GLU:HG2	5:A:830:HOH:O	2.16	0.46
1:A:346:ARG:HG2	5:A:878:HOH:O	2.14	0.46
1:B:291:ASN:HB3	1:B:293:MET:HE1	1.96	0.46
1:A:107:SER:HA	1:A:121:PHE:CD2	2.51	0.46
1:A:281:ILE:HG23	1:A:285:LEU:HD12	1.97	0.46
1:B:39:PRO:HG3	1:B:337:PHE:HE1	1.81	0.46
1:A:99:LEU:HD21	1:B:36:ILE:HD13	1.97	0.46
1:A:71:GLN:NE2	1:A:71:GLN:CA	2.79	0.46
1:A:258:HIS:ND1	1:A:297:SER:HB3	2.30	0.46
1:A:242:ALA:CB	4:A:607:EDO:H12	2.45	0.46
1:A:51:LYS:HE2	1:A:319:LEU:C	2.36	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:226:PHE:CZ	1:A:339:GLU:HG3	2.49	0.46
1:A:170:VAL:HG23	5:A:617:HOH:O	2.14	0.46
1:A:294:ILE:CB	5:A:617:HOH:O	2.62	0.46
1:B:130:SER:OG	1:B:135:ILE:HB	2.15	0.46
1:B:27:LYS:HG3	1:B:33:ARG:C	2.34	0.46
1:A:135:ILE:O	1:A:185:SER:HB2	2.15	0.46
1:A:250:ILE:CD1	1:A:274:LEU:HA	2.46	0.46
1:A:168:ILE:HD12	1:A:299:LEU:HD21	1.97	0.46
1:B:33:ARG:NH1	1:B:243:THR:OG1	2.48	0.46
1:A:237:VAL:HG23	1:A:238:ALA:C	2.36	0.46
1:A:44:ARG:O	1:A:47:ASP:HB2	2.15	0.46
1:B:199:VAL:O	1:B:200:SER:C	2.53	0.46
1:A:216:CYS:SG	1:A:255:HIS:CE1	3.08	0.46
1:B:245:PRO:HB3	1:B:335:PRO:HD2	1.96	0.46
1:A:199:VAL:HG12	1:A:203:LEU:HD11	1.98	0.46
1:A:137:LEU:CD2	1:A:292:TYR:OH	2.63	0.46
1:B:314:GLN:HG2	1:B:316:VAL:HG23	1.96	0.46
1:B:207:LYS:HB2	1:B:308:TYR:CZ	2.50	0.46
1:A:323:GLY:HA3	5:A:676:HOH:O	2.16	0.46
1:B:33:ARG:CZ	1:B:332:TYR:CE2	2.99	0.46
1:B:245:PRO:O	1:B:246:PHE:HB2	2.14	0.46
1:B:123:PHE:HB2	1:B:191:ALA:HB3	1.97	0.46
1:A:345:MET:HA	1:A:348:VAL:HG23	1.96	0.46
1:A:30:VAL:HG21	1:A:218:LEU:HD11	1.98	0.46
1:A:262:LEU:CD1	1:A:266:LYS:CB	2.94	0.46
1:B:180:ALA:HA	3:B:602:AMP:O2P	2.15	0.46
1:B:153:LYS:HG3	1:B:260:HIS:O	2.16	0.46
1:A:124:HIS:CD2	1:A:190:MET:SD	3.09	0.46
1:A:226:PHE:CE2	1:A:339:GLU:HG3	2.51	0.46
1:B:66:CYS:SG	1:B:133:HIS:HB2	2.55	0.46
1:B:81:PRO:HB2	1:B:84:ASP:CB	2.46	0.46
1:A:106:GLN:CA	1:A:106:GLN:OE1	2.63	0.46
1:B:165:ILE:HG22	1:B:166:ASN:H	1.79	0.46
1:A:25:LEU:HA	1:A:35:VAL:O	2.15	0.46
1:B:100:SER:HB3	1:B:103:LEU:HG	1.96	0.46
1:B:218:LEU:HB3	1:B:251:ILE:HG21	1.98	0.46
1:A:285:LEU:O	1:A:286:ASN:HB2	2.15	0.46
1:A:27:LYS:HB2	1:A:34:TRP:CD2	2.50	0.46
1:B:93:GLU:HG2	1:B:101:ARG:NH2	2.31	0.46
1:B:345:MET:HA	1:B:348:VAL:HG23	1.97	0.46
1:A:186:HIS:CD2	3:A:601:AMP:H5'2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:177:SER:OG	1:A:318:GLN:OE1	2.24	0.46
1:A:324:GLY:N	1:B:291:ASN:ND2	2.62	0.46
1:A:162:HIS:N	1:A:162:HIS:CD2	2.83	0.46
1:A:285:LEU:O	1:A:288:PRO:HD3	2.16	0.46
1:A:30:VAL:HG21	1:A:249:TRP:CH2	2.51	0.46
1:B:169:GLN:N	1:B:190:MET:O	2.41	0.46
1:B:322:VAL:HB	1:B:326:GLU:CD	2.37	0.46
1:A:196:PRO:HB2	1:B:329:THR:HB	1.98	0.46
1:A:79:ARG:HG3	1:A:79:ARG:O	2.16	0.46
1:A:116:ARG:O	1:B:26:ARG:HA	2.16	0.46
1:A:263:ASP:OD2	1:A:266:LYS:HG3	2.16	0.46
1:B:218:LEU:HD22	1:B:251:ILE:HD13	1.97	0.46
1:B:89:LEU:HD23	5:B:658:HOH:O	2.15	0.46
1:A:210:PHE:HA	1:A:215:LYS:O	2.16	0.46
1:A:297:SER:HB2	1:A:301:VAL:HB	1.97	0.46
1:B:101:ARG:NH2	1:B:124:HIS:H	2.14	0.46
1:A:336:VAL:HG11	1:A:341:VAL:HG23	1.98	0.46
1:A:255:HIS:HA	1:A:310:HIS:CE1	2.51	0.46
1:B:242:ALA:CB	4:B:610:EDO:H11	2.46	0.46
1:A:155:ARG:HB3	1:A:189:MET:HE1	1.97	0.45
1:A:94:ASN:O	1:A:97:PRO:HD3	2.17	0.45
1:A:301:VAL:CG2	1:A:305:GLN:HB2	2.46	0.45
1:A:33:ARG:NH2	5:A:652:HOH:O	2.48	0.45
1:B:288:PRO:HD2	5:B:628:HOH:O	2.16	0.45
1:A:197:PRO:HD3	5:B:784:HOH:O	2.15	0.45
1:B:172:LYS:NZ	1:B:186:HIS:O	2.49	0.45
1:B:320:SER:OG	1:B:321:GLY:N	2.48	0.45
1:A:117:THR:OG1	1:B:26:ARG:HG2	2.16	0.45
1:A:318:GLN:HG3	4:A:609:EDO:O1	2.16	0.45
1:B:252:PRO:HG3	1:B:311:TRP:CE2	2.51	0.45
1:B:252:PRO:HD2	1:B:311:TRP:O	2.16	0.45
1:B:289:PRO:HD2	1:B:318:GLN:HB3	1.98	0.45
1:A:249:TRP:CD1	1:A:314:GLN:CG	2.98	0.45
1:B:129:GLU:OE2	1:B:172:LYS:NZ	2.48	0.45
1:A:203:LEU:HD11	1:A:298:PRO:HG2	1.98	0.45
1:B:137:LEU:CB	1:B:172:LYS:HE2	2.45	0.45
1:B:75:PRO:O	1:B:93:GLU:HG3	2.16	0.45
1:A:74:ALA:HB3	1:A:93:GLU:O	2.17	0.45
1:B:291:ASN:O	1:B:293:MET:SD	2.75	0.45
1:B:209:TYR:CE2	1:B:213:THR:HG21	2.50	0.45
1:A:259:PHE:CD1	1:A:294:ILE:HD13	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:137:LEU:HD22	1:B:172:LYS:HD2	1.99	0.45
1:A:324:GLY:N	1:B:173:ASN:OD1	2.47	0.45
1:A:216:CYS:CB	1:A:219:CYS:SG	3.04	0.45
1:A:235:VAL:HG13	1:A:235:VAL:O	2.16	0.45
1:B:275:LYS:HD3	5:B:629:HOH:O	2.15	0.45
1:A:24:GLU:HG3	1:B:117:THR:HG23	1.97	0.45
1:A:280:LYS:HE2	1:A:350:LEU:CD1	2.46	0.45
1:A:156:ILE:HG13	1:A:189:MET:CE	2.47	0.45
1:A:322:VAL:HB	1:A:326:GLU:CD	2.36	0.45
1:B:222:LYS:HG2	5:B:836:HOH:O	2.15	0.45
1:A:234:PHE:CE1	1:A:270:LEU:HB2	2.51	0.45
1:B:228:ILE:HG12	1:B:342:ALA:CA	2.37	0.45
1:A:66:CYS:HB2	1:A:69:ARG:HD3	1.98	0.45
1:B:236:SER:H	1:B:273:LEU:HD21	1.80	0.45
1:A:218:LEU:HD23	1:A:218:LEU:HA	1.68	0.45
1:A:77:LEU:HD13	1:A:155:ARG:CZ	2.46	0.45
1:B:49:LYS:HD3	1:B:286:ASN:OD1	2.16	0.45
1:B:289:PRO:HB2	1:B:318:GLN:HE21	1.80	0.45
1:A:162:HIS:HB3	1:A:164:SER:OG	2.16	0.45
1:A:210:PHE:HB2	1:A:308:TYR:HB3	1.96	0.45
1:B:239:PRO:O	1:B:338:PRO:HB3	2.17	0.45
1:A:86:ASN:ND2	5:A:713:HOH:O	2.49	0.45
1:B:37:PHE:CE2	1:B:241:ALA:HA	2.52	0.45
1:B:63:CYS:SG	1:B:133:HIS:CE1	3.09	0.45
1:A:29:PRO:HB3	1:A:205:GLY:O	2.16	0.45
1:B:162:HIS:C	1:B:164:SER:H	2.20	0.45
1:A:258:HIS:HB3	1:A:260:HIS:ND1	2.30	0.45
1:A:242:ALA:CB	4:A:607:EDO:H11	2.47	0.45
1:B:102:ASN:O	5:B:701:HOH:O	2.21	0.45
1:A:106:GLN:O	1:A:107:SER:HB2	2.16	0.45
1:B:182:MET:HB2	1:B:186:HIS:NE2	2.31	0.45
1:B:67:ILE:C	1:B:67:ILE:HD12	2.35	0.45
1:A:207:LYS:O	1:A:211:GLU:HG3	2.17	0.45
1:A:332:TYR:HD2	1:A:332:TYR:N	2.14	0.45
1:A:313:LEU:C	1:A:313:LEU:HD23	2.37	0.45
1:A:154:LYS:O	1:A:158:GLN:HG3	2.16	0.45
1:B:244:TYR:CD1	4:B:612:EDO:H12	2.51	0.45
1:A:27:LYS:HG2	1:A:28:ASP:N	2.32	0.45
1:B:35:VAL:HG12	1:B:241:ALA:HB1	1.99	0.45
1:A:124:HIS:HA	1:A:189:MET:O	2.16	0.45
1:A:328:GLY:HA3	1:B:169:GLN:CD	2.37	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:33:ARG:HD2	5:B:646:HOH:O	2.16	0.45
1:B:133:HIS:HA	1:B:184:HIS:CE1	2.52	0.45
1:A:123:PHE:HB2	1:A:191:ALA:HB3	1.98	0.45
1:B:98:ALA:N	1:B:124:HIS:ND1	2.45	0.45
1:A:196:PRO:CG	1:B:329:THR:HB	2.47	0.45
1:B:342:ALA:O	1:B:346:ARG:HG3	2.17	0.45
1:A:290:TYR:CD2	1:A:290:TYR:C	2.90	0.45
1:A:169:GLN:CD	1:B:329:THR:HG23	2.35	0.45
1:A:118:ILE:CG1	1:B:25:LEU:HB2	2.47	0.45
1:A:77:LEU:HD12	1:A:91:VAL:HG12	1.99	0.45
1:A:248:ILE:O	1:A:314:GLN:HA	2.17	0.45
1:A:218:LEU:HD23	1:A:218:LEU:HA	1.75	0.45
1:B:333:ILE:HG22	1:B:333:ILE:O	2.15	0.45
1:B:24:GLU:O	1:B:36:ILE:HG23	2.17	0.45
1:B:67:ILE:HD12	1:B:68:GLY:H	1.80	0.45
1:A:78:PHE:HB3	5:A:780:HOH:O	2.17	0.45
1:B:320:SER:OG	5:B:773:HOH:O	2.21	0.45
1:A:77:LEU:C	1:A:78:PHE:HD2	2.21	0.45
1:A:209:TYR:CG	1:A:217:CYS:SG	3.10	0.45
1:A:156:ILE:HA	1:A:168:ILE:CD1	2.47	0.45
1:B:244:TYR:HB3	1:B:245:PRO:CD	2.47	0.45
1:A:295:HIS:NE2	1:A:314:GLN:OE1	2.42	0.45
1:B:203:LEU:HD11	1:B:298:PRO:HG2	1.99	0.45
1:B:302:THR:OG1	1:B:305:GLN:HG3	2.17	0.45
1:A:117:THR:HB	1:B:26:ARG:HG2	1.97	0.45
1:A:218:LEU:HA	1:A:218:LEU:HD23	1.71	0.45
1:B:143:VAL:HG23	5:B:723:HOH:O	2.17	0.45
1:A:26:ARG:HD3	1:A:240:PHE:CE2	2.52	0.45
1:A:252:PRO:CD	1:A:311:TRP:O	2.65	0.45
1:B:145:ILE:HD12	1:B:275:LYS:HB2	1.98	0.45
1:A:156:ILE:HG13	1:A:189:MET:CE	2.47	0.45
1:B:234:PHE:O	1:B:253:LYS:HE3	2.16	0.45
1:A:250:ILE:HD12	1:A:315:ILE:HD11	1.99	0.45
1:B:70:GLU:HA	5:B:715:HOH:O	2.16	0.45
1:A:132:VAL:CG1	1:A:135:ILE:HG13	2.47	0.45
1:B:255:HIS:HA	1:B:310:HIS:CE1	2.52	0.45
1:B:194:VAL:HB	5:B:738:HOH:O	2.16	0.45
1:A:64:PRO:O	1:A:73:CYS:SG	2.74	0.45
1:A:80:VAL:HB	1:A:89:LEU:HG	1.98	0.45
1:B:94:ASN:OD1	3:B:602:AMP:H1'	2.17	0.45
1:A:26:ARG:NH2	1:A:337:PHE:HD2	2.12	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:313:LEU:HD23	1:A:314:GLN:N	2.32	0.45
1:A:74:ALA:HB1	1:A:93:GLU:HB2	1.99	0.45
1:A:104:GLU:HB2	1:A:121:PHE:CE1	2.52	0.45
1:B:27:LYS:HG3	1:B:33:ARG:C	2.37	0.45
1:B:28:ASP:HB2	1:B:241:ALA:HB3	1.98	0.45
1:A:106:GLN:O	1:A:107:SER:HB2	2.17	0.45
1:A:78:PHE:CE1	1:A:154:LYS:HD3	2.52	0.45
1:A:333:ILE:O	1:A:333:ILE:HG22	2.17	0.45
1:A:141:ASP:O	1:A:144:GLY:N	2.50	0.45
1:A:77:LEU:O	1:A:78:PHE:HB3	2.17	0.45
1:A:65:PHE:CE2	1:A:126:VAL:HG11	2.50	0.44
1:A:137:LEU:HA	1:A:140:ILE:CD1	2.47	0.44
1:A:35:VAL:CA	1:A:331:CYS:SG	3.00	0.44
1:B:133:HIS:HA	1:B:184:HIS:ND1	2.32	0.44
1:A:219:CYS:O	1:A:220:GLU:HB3	2.16	0.44
1:B:67:ILE:HD12	1:B:68:GLY:H	1.82	0.44
1:A:64:PRO:O	1:A:73:CYS:SG	2.75	0.44
1:B:177:SER:CB	1:B:318:GLN:NE2	2.76	0.44
1:A:251:ILE:CD1	1:A:251:ILE:N	2.79	0.44
1:B:240:PHE:O	1:B:338:PRO:HG3	2.17	0.44
1:A:329:THR:HB	1:B:196:PRO:CG	2.47	0.44
1:A:171:PHE:CZ	1:A:188:GLN:HB2	2.51	0.44
1:B:170:VAL:HG22	1:B:189:MET:HG2	1.98	0.44
1:B:273:LEU:O	1:B:277:MET:HG2	2.17	0.44
1:B:172:LYS:HB2	1:B:187:SER:HB3	1.99	0.44
1:B:93:GLU:HG2	1:B:101:ARG:NH2	2.32	0.44
1:A:340:ASP:O	1:A:343:LYS:HB3	2.17	0.44
1:B:137:LEU:HB2	1:B:172:LYS:HE2	2.00	0.44
1:B:89:LEU:HD12	1:B:90:ARG:N	2.32	0.44
1:A:62:SER:HA	1:A:66:CYS:SG	2.58	0.44
1:A:149:LEU:HA	1:A:152:TYR:HD2	1.83	0.44
1:B:67:ILE:HG23	1:B:67:ILE:O	2.16	0.44
1:A:65:PHE:CD2	1:A:186:HIS:CD2	3.06	0.44
1:B:235:VAL:O	1:B:236:SER:C	2.56	0.44
1:B:25:LEU:HA	1:B:35:VAL:O	2.18	0.44
1:A:170:VAL:HG22	1:A:189:MET:HE2	1.99	0.44
1:A:101:ARG:O	1:A:104:GLU:HB2	2.18	0.44
1:A:61:SER:HB2	5:A:839:HOH:O	2.17	0.44
1:B:100:SER:OG	1:B:103:LEU:HG	2.17	0.44
1:B:219:CYS:SG	1:B:255:HIS:HB2	2.57	0.44
1:B:216:CYS:SG	1:B:308:TYR:HA	2.58	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:90:ARG:HD3	5:B:793:HOH:O	2.17	0.44
1:B:48:PHE:HB2	1:B:246:PHE:CE1	2.53	0.44
1:B:232:SER:H	1:B:269:ASP:CG	2.17	0.44
1:A:325:PHE:CD2	1:A:333:ILE:HD11	2.52	0.44
5:A:737:HOH:O	1:B:117:THR:CG2	2.65	0.44
1:B:121:PHE:O	1:B:193:PRO:HD3	2.16	0.44
1:A:79:ARG:O	1:A:82:ASP:HA	2.17	0.44
1:A:186:HIS:CE1	3:A:601:AMP:P	3.10	0.44
1:B:226:PHE:O	1:B:237:VAL:HA	2.18	0.44
1:A:98:ALA:HB3	1:A:190:MET:CE	2.46	0.44
1:B:289:PRO:HG3	5:B:737:HOH:O	2.17	0.44
1:A:263:ASP:OD2	1:A:265:VAL:N	2.49	0.44
1:A:199:VAL:HG12	1:A:203:LEU:CD1	2.47	0.44
1:B:239:PRO:O	1:B:242:ALA:HB2	2.18	0.44
1:B:26:ARG:HD3	1:B:240:PHE:CE2	2.52	0.44
1:B:65:PHE:HE2	1:B:186:HIS:ND1	2.15	0.44
1:A:88:LYS:HD2	5:A:713:HOH:O	2.17	0.44
1:B:48:PHE:HD2	1:B:319:LEU:HD13	1.83	0.44
1:B:305:GLN:C	1:B:307:PRO:HD2	2.37	0.44
1:B:228:ILE:HG22	1:B:229:ASP:N	2.32	0.44
1:A:168:ILE:HG21	1:A:189:MET:CE	2.47	0.44
1:A:77:LEU:O	1:A:78:PHE:HB3	2.18	0.44
1:B:180:ALA:HA	3:B:602:AMP:O2P	2.17	0.44
1:A:227:VAL:HG12	1:A:228:ILE:N	2.32	0.44
1:A:251:ILE:HA	1:A:252:PRO:HD3	1.90	0.44
1:A:330:GLY:HA3	1:B:197:PRO:HB2	2.00	0.44
1:A:324:GLY:H	1:B:291:ASN:ND2	2.16	0.44
1:B:222:LYS:NZ	5:B:813:HOH:O	2.33	0.44
1:A:196:PRO:HG2	1:A:199:VAL:HG23	2.00	0.44
1:B:123:PHE:O	1:B:190:MET:HA	2.17	0.44
5:A:764:HOH:O	1:B:23:PRO:HG3	2.17	0.44
1:A:145:ILE:O	1:A:146:GLY:C	2.56	0.44
1:A:207:LYS:O	1:A:211:GLU:HG3	2.18	0.44
1:A:227:VAL:CG1	1:A:228:ILE:N	2.81	0.44
1:B:181:SER:HG	3:B:602:AMP:P	2.41	0.44
1:A:328:GLY:CA	1:B:293:MET:HG2	2.48	0.44
1:B:292:TYR:HE1	1:B:313:LEU:HD11	1.83	0.44
1:A:63:CYS:HB2	1:A:64:PRO:CD	2.48	0.44
1:A:323:GLY:HA3	5:A:677:HOH:O	2.18	0.44
1:B:196:PRO:HA	1:B:197:PRO:HD3	1.89	0.44
1:B:70:GLU:HG3	1:B:90:ARG:NH1	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:325:PHE:O	1:B:329:THR:HG23	2.18	0.44
1:B:21:GLN:HG2	1:B:22:SER:N	2.32	0.44
1:B:80:VAL:HA	1:B:81:PRO:C	2.37	0.44
1:B:250:ILE:HB	1:B:313:LEU:HB3	2.00	0.44
1:A:239:PRO:O	1:A:240:PHE:C	2.56	0.44
1:B:177:SER:HB2	1:B:318:GLN:OE1	2.17	0.44
1:B:26:ARG:O	1:B:34:TRP:HA	2.17	0.44
1:A:266:LYS:HE3	5:A:805:HOH:O	2.18	0.44
1:A:101:ARG:NH1	1:A:102:ASN:OD1	2.50	0.44
1:A:243:THR:HG22	1:A:332:TYR:CD1	2.53	0.44
1:A:150:ILE:CG2	5:A:663:HOH:O	2.66	0.44
1:A:118:ILE:HD11	1:A:193:PRO:HG2	2.00	0.44
1:A:197:PRO:HD3	5:B:786:HOH:O	2.18	0.44
1:A:48:PHE:CE2	1:A:336:VAL:HG22	2.53	0.44
1:A:196:PRO:CB	1:B:329:THR:HB	2.47	0.44
1:B:28:ASP:HB2	1:B:241:ALA:HB3	1.99	0.44
1:B:280:LYS:O	1:B:281:ILE:C	2.56	0.44
1:A:288:PRO:HD2	5:A:642:HOH:O	2.18	0.44
1:B:173:ASN:ND2	1:B:291:ASN:ND2	2.66	0.44
1:A:137:LEU:HD11	1:A:145:ILE:HG12	2.00	0.44
1:B:27:LYS:HG2	1:B:28:ASP:H	1.83	0.44
1:A:117:THR:HA	1:B:25:LEU:O	2.18	0.44
1:B:33:ARG:HH22	1:B:243:THR:CB	2.25	0.44
1:A:116:ARG:NH2	1:B:224:LYS:CD	2.81	0.44
1:B:87:TRP:CE3	1:B:90:ARG:HG3	2.53	0.44
1:B:283:LYS:HB2	5:B:773:HOH:O	2.17	0.44
1:B:184:HIS:O	1:B:186:HIS:CD2	2.71	0.44
1:A:50:SER:N	1:A:285:LEU:O	2.45	0.44
1:B:50:SER:HA	1:B:288:PRO:HB3	2.00	0.44
1:B:104:GLU:O	1:B:107:SER:N	2.51	0.44
1:B:244:TYR:HA	5:B:617:HOH:O	2.17	0.44
1:A:46:THR:HB	1:A:344:VAL:CG2	2.47	0.44
1:A:301:VAL:HG22	1:A:302:THR:N	2.32	0.44
1:B:338:PRO:HA	1:B:341:VAL:HG23	1.99	0.44
1:B:50:SER:HB2	1:B:288:PRO:HB3	1.99	0.44
1:A:329:THR:O	1:B:197:PRO:HD2	2.18	0.44
1:A:27:LYS:HB2	1:A:34:TRP:CZ3	2.53	0.44
1:A:118:ILE:HG23	1:B:34:TRP:CH2	2.53	0.44
1:B:276:LEU:O	1:B:279:GLN:N	2.51	0.44
1:B:292:TYR:C	1:B:292:TYR:CD1	2.91	0.43
1:B:74:ALA:HB3	1:B:93:GLU:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:72:GLU:OE1	5:A:772:HOH:O	2.21	0.43
1:B:229:ASP:OD1	5:B:663:HOH:O	2.21	0.43
1:B:228:ILE:O	1:B:346:ARG:HG2	2.18	0.43
1:A:228:ILE:HD12	1:A:248:ILE:HG23	2.00	0.43
1:B:225:HIS:HB3	1:B:237:VAL:HB	2.00	0.43
1:A:81:PRO:HD2	1:A:87:TRP:HA	2.00	0.43
1:A:82:ASP:OD1	1:A:83:HIS:ND1	2.35	0.43
1:A:123:PHE:CD2	1:A:159:ILE:HG23	2.53	0.43
1:A:232:SER:N	1:A:269:ASP:OD1	2.47	0.43
1:B:34:TRP:N	5:B:786:HOH:O	2.51	0.43
1:B:264:ASP:O	1:B:267:ALA:HB3	2.17	0.43
1:A:256:SER:O	1:A:310:HIS:CD2	2.71	0.43
1:A:116:ARG:CD	5:A:822:HOH:O	2.55	0.43
1:A:203:LEU:HD11	1:A:298:PRO:HG2	1.99	0.43
1:B:295:HIS:O	1:B:311:TRP:HB2	2.18	0.43
1:A:197:PRO:O	1:A:201:SER:CB	2.66	0.43
1:B:104:GLU:HA	1:B:121:PHE:CD1	2.53	0.43
1:A:37:PHE:CD1	1:A:334:ASN:HB3	2.53	0.43
1:B:154:LYS:HE2	5:B:718:HOH:O	2.16	0.43
1:A:100:SER:HB3	1:A:103:LEU:HG	2.00	0.43
1:A:87:TRP:CH2	1:A:131:PRO:HA	2.53	0.43
1:A:172:LYS:CG	1:A:173:ASN:N	2.80	0.43
1:A:237:VAL:O	1:A:249:TRP:N	2.50	0.43
1:A:249:TRP:NE1	1:A:314:GLN:HG3	2.33	0.43
1:A:206:THR:HB	1:A:308:TYR:HB2	2.00	0.43
1:A:89:LEU:HB2	1:A:128:ILE:O	2.18	0.43
1:A:257:SER:HA	1:A:309:THR:HG22	2.01	0.43
1:B:94:ASN:HB2	1:B:124:HIS:O	2.18	0.43
1:B:190:MET:CG	1:B:192:LEU:HD21	2.49	0.43
1:A:243:THR:HG23	1:A:332:TYR:CG	2.53	0.43
1:B:300:LYS:NZ	5:B:738:HOH:O	2.43	0.43
1:A:336:VAL:O	1:A:337:PHE:C	2.55	0.43
1:A:239:PRO:HD2	1:A:247:GLU:O	2.18	0.43
1:A:198:THR:HG23	1:B:330:GLY:N	2.32	0.43
1:A:198:THR:OG1	1:B:329:THR:CA	2.65	0.43
1:B:129:GLU:OE1	1:B:186:HIS:O	2.35	0.43
1:B:66:CYS:SG	1:B:133:HIS:HB2	2.59	0.43
1:B:206:THR:OG1	1:B:308:TYR:HD2	2.02	0.43
1:A:152:TYR:OH	1:A:292:TYR:OH	2.37	0.43
1:B:69:ARG:HD2	1:B:72:GLU:OE2	2.19	0.43
1:A:216:CYS:O	1:A:219:CYS:SG	2.69	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:129:GLU:OE1	1:A:187:SER:HB3	2.19	0.43
1:B:31:THR:HG21	5:B:659:HOH:O	2.17	0.43
1:B:276:LEU:HD23	1:B:277:MET:HE2	2.01	0.43
1:A:116:ARG:CD	5:A:820:HOH:O	2.47	0.43
1:B:165:ILE:CG2	1:B:166:ASN:N	2.80	0.43
1:B:172:LYS:O	1:B:291:ASN:HA	2.17	0.43
1:B:37:PHE:CZ	1:B:338:PRO:HD3	2.54	0.43
1:A:343:LYS:HZ2	1:A:344:VAL:HG23	1.83	0.43
1:A:138:SER:O	1:A:275:LYS:HG3	2.19	0.43
1:B:203:LEU:O	1:B:204:ASP:C	2.57	0.43
1:A:95:LEU:HG	1:A:96:TYR:CZ	2.53	0.43
1:A:73:CYS:SG	1:A:90:ARG:NH1	2.92	0.43
1:A:118:ILE:HG23	1:B:34:TRP:HH2	1.83	0.43
1:A:39:PRO:HG2	1:A:337:PHE:CE1	2.53	0.43
1:A:323:GLY:O	1:A:327:ILE:HG13	2.19	0.43
1:A:292:TYR:CD1	1:A:292:TYR:C	2.91	0.43
1:B:227:VAL:HA	1:B:237:VAL:HG12	2.00	0.43
1:A:186:HIS:CD2	3:A:601:AMP:H5'2	2.53	0.43
1:A:243:THR:CG2	1:A:332:TYR:CD1	3.02	0.43
1:A:30:VAL:HG13	1:A:202:ARG:HD3	2.00	0.43
1:B:313:LEU:HD21	1:B:315:ILE:HG13	2.01	0.43
1:A:91:VAL:HG22	1:A:127:VAL:HG22	2.00	0.43
1:A:67:ILE:CD1	1:A:86:ASN:HA	2.47	0.43
1:B:105:THR:HG23	5:B:701:HOH:O	2.18	0.43
1:A:198:THR:O	1:A:202:ARG:HB2	2.19	0.43
1:A:126:VAL:CG1	1:A:128:ILE:HG13	2.46	0.43
1:B:243:THR:HG23	1:B:332:TYR:CG	2.53	0.43
1:B:310:HIS:HD2	1:B:311:TRP:N	2.17	0.43
1:B:77:LEU:O	1:B:78:PHE:HB3	2.18	0.43
1:A:44:ARG:CG	1:A:46:THR:HG22	2.48	0.43
1:A:236:SER:OG	1:A:277:MET:CE	2.66	0.43
1:B:322:VAL:CG1	1:B:326:GLU:HG2	2.47	0.43
1:A:162:HIS:C	1:A:164:SER:N	2.72	0.43
1:A:89:LEU:C	1:A:89:LEU:HD12	2.38	0.43
1:B:207:LYS:HB2	1:B:308:TYR:CE1	2.53	0.43
1:B:280:LYS:HB2	1:B:345:MET:HE1	2.00	0.43
1:A:329:THR:HB	1:B:196:PRO:HB2	2.00	0.43
1:B:48:PHE:HB2	1:B:246:PHE:HE1	1.83	0.43
1:A:281:ILE:N	1:A:345:MET:HE1	2.34	0.43
1:A:313:LEU:C	1:A:313:LEU:HD23	2.39	0.43
1:B:234:PHE:CD2	1:B:252:PRO:HA	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:46:THR:N	1:B:344:VAL:HG21	2.34	0.43
1:B:163:ASP:O	1:B:163:ASP:OD1	2.37	0.43
1:B:48:PHE:CD2	1:B:319:LEU:HD13	2.54	0.43
1:A:168:ILE:HD12	1:A:299:LEU:HD21	2.00	0.43
1:A:336:VAL:HG12	1:A:341:VAL:HG23	2.01	0.43
1:A:288:PRO:C	1:A:289:PRO:O	2.56	0.43
1:A:184:HIS:O	1:A:186:HIS:CE1	2.72	0.43
1:B:338:PRO:HG2	1:B:339:GLU:OE1	2.19	0.43
1:B:141:ASP:OD2	1:B:143:VAL:HG13	2.18	0.43
1:A:198:THR:HB	4:A:608:EDO:O1	2.19	0.43
1:B:222:LYS:NZ	1:B:235:VAL:HB	2.33	0.43
1:B:228:ILE:HG23	1:B:346:ARG:HG3	2.01	0.43
3:A:601:AMP:H8	5:A:672:HOH:O	2.01	0.43
1:A:197:PRO:HD2	1:B:329:THR:O	2.19	0.43
1:A:220:GLU:HG3	1:A:220:GLU:O	2.17	0.43
1:B:173:ASN:OD1	1:B:291:ASN:ND2	2.49	0.43
1:B:76:GLU:HA	1:B:92:ILE:HG22	2.00	0.43
1:B:248:ILE:CD1	1:B:345:MET:HE2	2.40	0.43
1:A:329:THR:C	1:A:331:CYS:N	2.72	0.43
1:A:318:GLN:HG3	4:A:609:EDO:O1	2.19	0.43
1:A:229:ASP:O	1:A:236:SER:N	2.51	0.43
1:A:306:LEU:N	1:A:307:PRO:CD	2.81	0.43
1:A:243:THR:HG22	1:A:243:THR:O	2.18	0.43
1:B:222:LYS:NZ	1:B:253:LYS:HE2	2.34	0.43
1:A:173:ASN:ND2	1:A:188:GLN:NE2	2.67	0.43
1:A:182:MET:CG	3:A:601:AMP:H5'1	2.49	0.43
1:A:132:VAL:HG11	1:A:135:ILE:HG13	2.01	0.43
1:A:140:ILE:CG2	1:A:141:ASP:N	2.82	0.43
1:B:210:PHE:HB2	1:B:308:TYR:HB3	1.99	0.43
1:B:104:GLU:CD	1:B:162:HIS:HD1	2.22	0.43
1:B:279:GLN:HB3	1:B:350:LEU:HD21	2.00	0.43
1:A:265:VAL:HG23	5:A:808:HOH:O	2.19	0.43
1:A:136:GLN:O	1:A:137:LEU:C	2.57	0.43
1:B:246:PHE:HB2	1:B:319:LEU:CD1	2.48	0.43
1:A:23:PRO:O	1:A:24:GLU:HG3	2.18	0.43
1:B:306:LEU:N	1:B:307:PRO:CD	2.82	0.43
1:A:91:VAL:HG22	1:A:127:VAL:HG22	2.00	0.43
1:A:96:TYR:CE2	5:A:847:HOH:O	2.56	0.43
1:A:244:TYR:HB3	5:A:621:HOH:O	2.19	0.43
1:B:292:TYR:HB2	1:B:313:LEU:CD2	2.49	0.43
1:B:231:SER:C	1:B:233:HIS:N	2.72	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:228:ILE:HB	1:A:236:SER:OG	2.19	0.43
1:B:152:TYR:O	1:B:156:ILE:HG13	2.19	0.43
1:B:289:PRO:HG2	1:B:318:GLN:HE21	1.84	0.43
1:A:325:PHE:HB2	1:B:171:PHE:CZ	2.54	0.43
1:A:186:HIS:CD2	3:A:601:AMP:H5'1	2.54	0.43
1:B:306:LEU:HB2	1:B:307:PRO:HD3	2.01	0.43
1:A:152:TYR:CD2	1:A:170:VAL:HG11	2.54	0.43
1:B:268:VAL:O	1:B:271:GLY:HA3	2.19	0.42
1:B:29:PRO:HB3	1:B:209:TYR:HB2	2.01	0.42
1:B:130:SER:C	1:B:132:VAL:H	2.23	0.42
1:B:99:LEU:HD12	1:B:190:MET:SD	2.59	0.42
1:B:276:LEU:HD23	1:B:277:MET:CE	2.49	0.42
1:B:62:SER:HA	1:B:66:CYS:SG	2.59	0.42
1:A:258:HIS:HE1	1:A:301:VAL:HG11	1.84	0.42
1:B:276:LEU:O	1:B:280:LYS:N	2.45	0.42
1:B:171:PHE:CE1	1:B:188:GLN:HB2	2.54	0.42
1:B:326:GLU:HG3	1:B:331:CYS:O	2.19	0.42
1:B:210:PHE:O	1:B:214:GLY:HA2	2.18	0.42
1:A:129:GLU:OE2	1:A:185:SER:OG	2.36	0.42
1:B:46:THR:N	1:B:336:VAL:HG13	2.34	0.42
1:A:264:ASP:HB2	5:A:805:HOH:O	2.18	0.42
1:A:35:VAL:HG23	1:A:332:TYR:HB2	2.01	0.42
1:B:296:THR:HA	1:B:311:TRP:HB2	2.01	0.42
1:B:95:LEU:HB2	3:B:602:AMP:C2	2.54	0.42
1:B:226:PHE:HB2	1:B:238:ALA:HB3	2.02	0.42
1:A:168:ILE:HG23	1:A:190:MET:C	2.39	0.42
1:B:97:PRO:HB2	1:B:99:LEU:O	2.19	0.42
1:A:244:TYR:OH	1:B:327:ILE:HG23	2.18	0.42
1:A:23:PRO:HA	1:A:37:PHE:O	2.20	0.42
1:A:168:ILE:HG12	1:A:191:ALA:CB	2.50	0.42
1:A:89:LEU:HB2	1:A:128:ILE:O	2.19	0.42
1:A:255:HIS:HA	1:A:310:HIS:HD1	1.84	0.42
1:A:216:CYS:SG	1:A:255:HIS:ND1	2.87	0.42
1:A:305:GLN:HA	1:A:308:TYR:CZ	2.54	0.42
1:B:101:ARG:NH2	1:B:123:PHE:HD1	2.17	0.42
1:A:225:HIS:ND1	1:A:239:PRO:HA	2.34	0.42
1:A:88:LYS:HE3	5:A:713:HOH:O	2.19	0.42
1:B:232:SER:HB2	5:B:621:HOH:O	2.18	0.42
1:A:194:VAL:O	1:A:195:VAL:C	2.58	0.42
1:A:190:MET:HE2	1:B:325:PHE:CE1	2.53	0.42
1:B:37:PHE:CE1	1:B:336:VAL:O	2.72	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:63:CYS:SG	1:B:64:PRO:N	2.92	0.42
1:B:104:GLU:OE2	1:B:162:HIS:ND1	2.52	0.42
1:A:256:SER:O	1:A:310:HIS:HA	2.20	0.42
1:A:224:LYS:CE	5:A:880:HOH:O	2.46	0.42
1:B:63:CYS:HB2	1:B:64:PRO:CD	2.49	0.42
1:B:228:ILE:O	1:B:229:ASP:CG	2.58	0.42
1:A:170:VAL:HB	1:A:294:ILE:HB	2.01	0.42
1:B:100:SER:O	1:B:121:PHE:HA	2.19	0.42
1:B:199:VAL:O	1:B:200:SER:C	2.58	0.42
1:B:80:VAL:CG2	1:B:89:LEU:HD11	2.49	0.42
1:A:337:PHE:HB3	1:A:339:GLU:CD	2.36	0.42
1:B:226:PHE:HB3	1:B:342:ALA:CB	2.49	0.42
1:A:147:ASP:O	1:A:148:ILE:C	2.57	0.42
1:B:65:PHE:CD1	1:B:128:ILE:HD11	2.55	0.42
1:B:106:GLN:HB3	1:B:119:VAL:HG11	2.01	0.42
1:A:80:VAL:HB	1:A:89:LEU:HG	2.01	0.42
1:B:160:ALA:HA	1:B:299:LEU:CD1	2.47	0.42
1:A:234:PHE:CE1	1:A:270:LEU:HB2	2.55	0.42
1:A:127:VAL:O	1:A:186:HIS:HB2	2.18	0.42
1:A:65:PHE:HB2	1:A:184:HIS:CD2	2.54	0.42
1:B:170:VAL:HG22	1:B:189:MET:HE2	2.00	0.42
1:A:196:PRO:CB	1:B:329:THR:HB	2.50	0.42
1:A:186:HIS:CD2	3:A:601:AMP:O1P	2.70	0.42
1:B:64:PRO:HD3	5:B:792:HOH:O	2.20	0.42
1:A:72:GLU:HG2	5:A:773:HOH:O	2.19	0.42
1:B:80:VAL:HA	1:B:81:PRO:C	2.39	0.42
1:A:51:LYS:CE	1:A:320:SER:HA	2.49	0.42
1:A:97:PRO:O	1:A:98:ALA:C	2.56	0.42
1:A:240:PHE:CE2	1:B:116:ARG:HB2	2.54	0.42
1:A:140:ILE:CG2	1:A:144:GLY:HA3	2.50	0.42
1:A:27:LYS:HD2	1:A:34:TRP:CE2	2.54	0.42
1:A:100:SER:HB3	1:A:103:LEU:HG	2.00	0.42
1:A:152:TYR:HA	1:A:189:MET:HE1	2.02	0.42
1:A:129:GLU:OE2	1:A:172:LYS:NZ	2.39	0.42
1:A:48:PHE:O	1:A:49:LYS:HD3	2.18	0.42
1:A:33:ARG:NH2	1:A:33:ARG:HG2	2.34	0.42
1:B:49:LYS:CD	1:B:286:ASN:OD1	2.68	0.42
1:A:229:ASP:OD2	1:A:276:LEU:HD21	2.20	0.42
1:B:172:LYS:HG2	1:B:173:ASN:N	2.34	0.42
1:A:177:SER:HB2	1:A:318:GLN:OE1	2.20	0.42
1:A:82:ASP:C	1:A:84:ASP:H	2.22	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:278:LEU:HB3	5:B:639:HOH:O	2.20	0.42
1:A:167:TYR:CD2	1:A:199:VAL:HG11	2.55	0.42
1:B:171:PHE:HB3	1:B:293:MET:HG3	2.02	0.42
1:A:280:LYS:C	1:A:345:MET:HE1	2.39	0.42
1:A:171:PHE:CE1	1:B:325:PHE:HB2	2.54	0.42
1:A:273:LEU:O	1:A:277:MET:HG2	2.19	0.42
1:B:180:ALA:HA	3:B:602:AMP:O2P	2.19	0.42
1:A:170:VAL:HB	1:A:294:ILE:HB	2.01	0.42
1:A:245:PRO:HA	4:A:607:EDO:O2	2.19	0.42
1:B:165:ILE:C	1:B:299:LEU:HD12	2.39	0.42
1:A:156:ILE:HG13	1:A:189:MET:HE1	2.02	0.42
1:A:246:PHE:CG	1:A:285:LEU:HD11	2.55	0.42
1:B:262:LEU:CD1	1:B:266:LYS:HB2	2.47	0.42
1:B:217:CYS:HB2	1:B:224:LYS:CE	2.36	0.42
1:B:121:PHE:CG	1:B:122:GLY:N	2.88	0.42
1:A:198:THR:HG23	1:B:329:THR:O	2.19	0.42
1:A:145:ILE:HG22	1:A:271:GLY:HA2	2.01	0.42
1:A:116:ARG:CB	1:A:116:ARG:CZ	2.90	0.42
1:A:27:LYS:HG3	1:A:33:ARG:O	2.19	0.42
1:B:81:PRO:HD3	1:B:88:LYS:HG3	2.02	0.42
1:B:297:SER:HA	1:B:298:PRO:HD3	1.95	0.42
1:B:200:SER:HB3	5:B:740:HOH:O	2.19	0.42
1:B:123:PHE:O	1:B:190:MET:HA	2.19	0.42
1:A:33:ARG:HG3	1:A:33:ARG:O	2.20	0.42
1:B:242:ALA:CB	4:B:610:EDO:H12	2.50	0.42
1:A:124:HIS:CD2	1:A:190:MET:HG2	2.55	0.42
1:A:197:PRO:HG3	1:B:33:ARG:HB2	2.00	0.42
1:B:170:VAL:HG13	1:B:189:MET:HG2	2.01	0.42
1:B:140:ILE:CG2	1:B:144:GLY:HA3	2.49	0.42
1:B:252:PRO:HG2	1:B:310:HIS:NE2	2.35	0.42
1:B:255:HIS:CE1	1:B:309:THR:O	2.72	0.42
1:A:202:ARG:NH1	1:A:296:THR:O	2.51	0.42
1:B:21:GLN:HB3	1:B:39:PRO:HG3	2.02	0.42
1:B:25:LEU:HD11	1:B:36:ILE:CG1	2.47	0.42
1:B:25:LEU:CD1	1:B:36:ILE:HG12	2.48	0.42
1:B:314:GLN:NE2	4:B:611:EDO:H22	2.35	0.42
1:B:252:PRO:HG2	1:B:310:HIS:CD2	2.53	0.42
1:B:81:PRO:HB2	1:B:84:ASP:HB2	2.02	0.42
1:A:26:ARG:HB3	1:A:241:ALA:HB2	2.01	0.42
1:A:31:THR:HA	5:A:668:HOH:O	2.20	0.42
1:B:302:THR:OG1	1:B:305:GLN:HG3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:129:GLU:OE1	1:A:186:HIS:C	2.57	0.42
1:B:47:ASP:OD1	1:B:48:PHE:N	2.53	0.42
1:B:129:GLU:OE1	1:B:172:LYS:HD2	2.20	0.42
1:B:98:ALA:O	1:B:99:LEU:HD23	2.20	0.42
1:B:100:SER:HB3	1:B:103:LEU:CG	2.50	0.42
1:B:95:LEU:HG	1:B:95:LEU:O	2.20	0.42
1:A:326:GLU:HG3	1:A:331:CYS:O	2.20	0.42
1:B:242:ALA:HB1	1:B:247:GLU:HB3	2.02	0.42
1:B:244:TYR:C	1:B:334:ASN:ND2	2.73	0.42
1:A:87:TRP:CH2	1:A:131:PRO:HA	2.54	0.42
1:A:100:SER:HB2	5:A:719:HOH:O	2.20	0.42
1:A:313:LEU:CD2	1:A:315:ILE:HG13	2.50	0.42
1:A:88:LYS:HE3	5:A:716:HOH:O	2.20	0.42
1:B:259:PHE:HA	1:B:311:TRP:CE2	2.55	0.42
1:B:106:GLN:HE21	1:B:119:VAL:HG11	1.84	0.42
1:B:101:ARG:NH1	1:B:124:HIS:H	2.14	0.42
1:A:301:VAL:HG22	1:A:302:THR:H	1.85	0.42
1:A:44:ARG:O	1:A:46:THR:N	2.53	0.42
1:B:259:PHE:CZ	1:B:262:LEU:HD22	2.55	0.42
1:B:49:LYS:HA	1:B:285:LEU:HA	2.02	0.42
1:A:44:ARG:CD	1:A:46:THR:HG22	2.50	0.42
1:B:154:LYS:NZ	5:B:718:HOH:O	2.49	0.42
1:A:274:LEU:O	1:A:278:LEU:HG	2.19	0.42
1:B:293:MET:N	1:B:314:GLN:O	2.44	0.42
1:A:264:ASP:O	1:A:267:ALA:HB3	2.20	0.42
1:B:255:HIS:NE2	1:B:306:LEU:O	2.47	0.42
1:A:121:PHE:C	1:A:121:PHE:CD1	2.93	0.42
1:B:243:THR:N	1:B:247:GLU:OE2	2.53	0.42
1:A:25:LEU:HB2	1:B:118:ILE:HG12	2.01	0.42
1:B:185:SER:O	1:B:186:HIS:HB3	2.19	0.42
1:B:80:VAL:HB	1:B:89:LEU:HG	2.02	0.42
1:B:256:SER:O	1:B:258:HIS:N	2.53	0.42
1:A:196:PRO:HG2	1:A:199:VAL:HG23	2.02	0.42
1:A:246:PHE:CE2	1:A:285:LEU:HD21	2.55	0.42
1:A:242:ALA:HA	5:A:622:HOH:O	2.20	0.42
1:B:289:PRO:CB	1:B:318:GLN:HE21	2.33	0.42
1:B:331:CYS:HG	1:B:332:TYR:N	2.15	0.42
1:A:44:ARG:HG3	1:A:45:PRO:HD2	2.02	0.42
1:A:38:SER:OG	1:B:98:ALA:HA	2.19	0.42
1:B:48:PHE:CZ	1:B:336:VAL:CG2	3.03	0.42
1:A:26:ARG:O	1:A:34:TRP:HA	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:127:VAL:HB	1:A:187:SER:CA	2.49	0.41
1:B:337:PHE:HB2	1:B:340:ASP:OD2	2.19	0.41
1:B:313:LEU:HD23	1:B:313:LEU:C	2.40	0.41
1:A:48:PHE:O	1:A:49:LYS:HD3	2.20	0.41
1:A:29:PRO:HB2	1:A:217:CYS:SG	2.59	0.41
1:B:153:LYS:HE3	5:B:731:HOH:O	2.19	0.41
1:A:236:SER:O	1:A:237:VAL:HG12	2.20	0.41
1:B:150:ILE:HG22	5:B:696:HOH:O	2.19	0.41
1:A:237:VAL:O	1:A:239:PRO:HD3	2.19	0.41
1:A:127:VAL:HG21	1:A:152:TYR:CE1	2.55	0.41
1:B:211:GLU:HA	5:B:749:HOH:O	2.19	0.41
1:B:234:PHE:CE1	1:B:270:LEU:HB2	2.55	0.41
1:B:171:PHE:HD1	1:B:173:ASN:OD1	2.03	0.41
1:A:281:ILE:HG23	1:A:285:LEU:HD12	2.02	0.41
1:A:276:LEU:HB3	1:A:277:MET:HE3	2.02	0.41
1:A:165:ILE:HG22	1:A:299:LEU:HD12	2.01	0.41
1:B:136:GLN:HG3	1:B:138:SER:OG	2.20	0.41
1:B:66:CYS:O	1:B:69:ARG:HB2	2.20	0.41
1:A:259:PHE:HD1	1:A:311:TRP:CZ2	2.38	0.41
1:B:265:VAL:HG23	5:B:672:HOH:O	2.20	0.41
1:B:313:LEU:CD2	1:B:315:ILE:HG13	2.50	0.41
1:B:47:ASP:OD1	1:B:48:PHE:HD1	2.02	0.41
1:A:44:ARG:HB3	1:A:47:ASP:CG	2.40	0.41
1:B:247:GLU:CD	1:B:249:TRP:HE1	2.24	0.41
1:A:188:GLN:NE2	3:A:601:AMP:H5'2	2.35	0.41
1:B:306:LEU:N	1:B:307:PRO:CD	2.83	0.41
1:B:258:HIS:HB3	1:B:260:HIS:ND1	2.35	0.41
1:A:349:SER:C	1:A:351:THR:H	2.23	0.41
1:A:153:LYS:HE3	1:A:260:HIS:O	2.21	0.41
1:B:231:SER:C	1:B:233:HIS:H	2.23	0.41
1:A:45:PRO:HB2	1:A:344:VAL:HG21	2.03	0.41
1:A:288:PRO:C	1:A:289:PRO:O	2.58	0.41
1:A:199:VAL:HG11	1:A:298:PRO:CG	2.51	0.41
1:B:252:PRO:CD	1:B:311:TRP:O	2.67	0.41
1:B:252:PRO:HG3	1:B:311:TRP:CE2	2.55	0.41
1:B:249:TRP:HA	1:B:313:LEU:O	2.20	0.41
1:A:50:SER:HB2	1:A:288:PRO:CB	2.46	0.41
1:A:196:PRO:HA	1:A:197:PRO:HD3	1.72	0.41
1:B:33:ARG:O	1:B:34:TRP:C	2.59	0.41
1:B:318:GLN:C	1:B:319:LEU:HD23	2.41	0.41
1:B:159:ILE:CG2	1:B:168:ILE:HD11	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:251:ILE:HG22	1:A:252:PRO:O	2.20	0.41
1:B:292:TYR:C	1:B:293:MET:CE	2.89	0.41
1:A:170:VAL:HB	1:A:294:ILE:HD12	2.02	0.41
1:A:318:GLN:NE2	4:A:609:EDO:O2	2.51	0.41
1:A:63:CYS:N	1:A:66:CYS:SG	2.93	0.41
1:A:293:MET:SD	1:A:293:MET:N	2.93	0.41
1:A:34:TRP:CD1	1:B:194:VAL:HG21	2.55	0.41
1:B:28:ASP:O	1:B:32:ASN:N	2.49	0.41
1:B:305:GLN:HB3	1:B:308:TYR:CZ	2.55	0.41
1:A:125:ASP:HB2	1:A:189:MET:HB2	2.03	0.41
1:A:175:GLY:O	1:A:178:ALA:N	2.46	0.41
1:B:27:LYS:HB2	1:B:34:TRP:CE3	2.55	0.41
1:B:226:PHE:HB3	1:B:342:ALA:HB2	2.02	0.41
1:B:304:SER:O	1:B:307:PRO:HD2	2.20	0.41
1:A:98:ALA:HB3	1:A:190:MET:SD	2.61	0.41
1:B:48:PHE:HB2	1:B:246:PHE:CZ	2.55	0.41
1:A:72:GLU:CG	5:A:772:HOH:O	2.68	0.41
1:B:100:SER:HB3	1:B:103:LEU:CD1	2.45	0.41
1:A:49:LYS:HD2	1:A:286:ASN:HD21	1.84	0.41
1:B:210:PHE:O	1:B:214:GLY:N	2.45	0.41
1:A:90:ARG:O	1:A:128:ILE:N	2.41	0.41
1:A:117:THR:HG23	1:B:26:ARG:HG2	2.02	0.41
1:B:80:VAL:HA	1:B:81:PRO:C	2.40	0.41
1:B:184:HIS:O	1:B:186:HIS:CD2	2.73	0.41
1:A:152:TYR:CG	1:A:170:VAL:HG11	2.55	0.41
1:B:76:GLU:OE1	1:B:79:ARG:HB3	2.20	0.41
1:A:290:TYR:HB3	1:A:317:PRO:HA	2.02	0.41
1:A:283:LYS:NZ	5:A:654:HOH:O	2.53	0.41
1:A:133:HIS:HA	1:A:184:HIS:ND1	2.35	0.41
1:B:87:TRP:CE3	1:B:90:ARG:HG3	2.55	0.41
1:A:152:TYR:HH	1:A:187:SER:CB	2.34	0.41
1:A:149:LEU:HA	1:A:149:LEU:HD23	1.81	0.41
1:B:153:LYS:HE3	5:B:737:HOH:O	2.20	0.41
1:B:327:ILE:O	1:B:329:THR:N	2.53	0.41
1:B:319:LEU:O	1:B:320:SER:O	2.38	0.41
1:B:333:ILE:O	1:B:335:PRO:HD3	2.20	0.41
1:A:313:LEU:HD12	1:A:314:GLN:H	1.86	0.41
1:A:327:ILE:HG21	1:B:293:MET:HE3	2.02	0.41
1:A:312:PHE:HZ	4:A:608:EDO:H12	1.86	0.41
1:B:234:PHE:HA	1:B:251:ILE:O	2.20	0.41
1:B:127:VAL:HB	1:B:187:SER:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:285:LEU:C	1:A:288:PRO:HD3	2.40	0.41
1:A:192:LEU:HD12	1:A:196:PRO:HD3	2.01	0.41
1:A:177:SER:OG	1:A:318:GLN:NE2	2.53	0.41
1:A:171:PHE:CE2	1:B:325:PHE:HB2	2.56	0.41
1:A:330:GLY:C	1:B:197:PRO:HG2	2.40	0.41
1:B:242:ALA:HB3	4:B:610:EDO:H21	2.03	0.41
1:A:39:PRO:HA	1:A:335:PRO:O	2.20	0.41
1:A:233:HIS:CA	1:A:253:LYS:HE2	2.50	0.41
1:A:237:VAL:O	1:A:248:ILE:HA	2.21	0.41
1:B:69:ARG:HD2	1:B:72:GLU:OE2	2.20	0.41
1:A:256:SER:O	1:A:311:TRP:N	2.53	0.41
1:A:65:PHE:CD1	1:A:65:PHE:N	2.89	0.41
1:A:250:ILE:HD12	1:A:274:LEU:HD13	2.02	0.41
1:B:218:LEU:HA	1:B:218:LEU:HD23	1.86	0.41
1:A:186:HIS:CD2	3:A:601:AMP:O1P	2.73	0.41
1:B:185:SER:CA	5:B:716:HOH:O	2.65	0.41
1:A:301:VAL:HG23	1:A:305:GLN:OE1	2.20	0.41
1:A:23:PRO:O	1:B:120:GLY:CA	2.65	0.41
1:A:257:SER:HA	1:A:309:THR:O	2.20	0.41
1:B:95:LEU:HD23	1:B:96:TYR:CE1	2.56	0.41
1:B:285:LEU:O	1:B:286:ASN:HB2	2.21	0.41
1:A:250:ILE:CD1	1:A:315:ILE:HD11	2.51	0.41
1:B:257:SER:O	1:B:297:SER:HB3	2.21	0.41
1:A:341:VAL:HG21	4:A:607:EDO:O1	2.21	0.41
1:A:236:SER:O	1:A:237:VAL:HG13	2.20	0.41
1:A:312:PHE:HE2	1:A:314:GLN:HB2	1.86	0.41
1:A:94:ASN:ND2	1:A:124:HIS:CD2	2.89	0.41
1:A:216:CYS:O	1:A:219:CYS:HB3	2.21	0.41
1:B:239:PRO:O	1:B:241:ALA:N	2.54	0.41
1:A:234:PHE:N	1:A:253:LYS:HG3	2.35	0.41
1:A:77:LEU:O	1:A:78:PHE:HB3	2.20	0.41
1:B:344:VAL:O	1:B:348:VAL:HG23	2.20	0.41
1:A:285:LEU:CB	1:A:288:PRO:HD3	2.50	0.41
1:A:213:THR:HB	1:A:215:LYS:HZ1	1.83	0.41
1:A:104:GLU:O	1:A:107:SER:N	2.52	0.41
1:A:27:LYS:HB2	1:A:34:TRP:CE3	2.56	0.41
1:A:323:GLY:CA	5:A:677:HOH:O	2.68	0.41
1:B:209:TYR:HH	1:B:224:LYS:HE3	1.86	0.41
1:B:327:ILE:O	1:B:328:GLY:C	2.57	0.41
1:A:215:LYS:HD2	1:A:220:GLU:OE1	2.21	0.41
1:B:251:ILE:HA	1:B:252:PRO:HD2	1.94	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:317:PRO:HB2	1:B:319:LEU:HG	2.02	0.41
1:A:166:ASN:CA	1:A:299:LEU:HD12	2.51	0.41
1:B:27:LYS:HG2	1:B:28:ASP:N	2.36	0.41
1:B:33:ARG:CZ	1:B:243:THR:OG1	2.69	0.41
1:A:116:ARG:HH22	1:B:224:LYS:CD	2.34	0.41
1:B:167:TYR:HE2	1:B:296:THR:O	2.04	0.41
1:A:69:ARG:HH21	1:A:72:GLU:CD	2.24	0.41
1:B:220:GLU:OE1	1:B:224:LYS:HE2	2.21	0.41
1:A:246:PHE:HA	1:A:341:VAL:CG1	2.51	0.41
1:B:63:CYS:O	1:B:69:ARG:HG3	2.20	0.41
1:B:244:TYR:CE1	4:B:612:EDO:H12	2.55	0.41
1:B:50:SER:OG	1:B:288:PRO:HB3	2.20	0.41
1:B:168:ILE:HG12	1:B:191:ALA:CB	2.51	0.41
1:A:86:ASN:C	5:A:711:HOH:O	2.59	0.41
1:A:136:GLN:O	1:A:139:ASP:HB2	2.21	0.41
1:A:227:VAL:O	1:A:346:ARG:NE	2.47	0.41
1:A:233:HIS:CG	1:A:266:LYS:HG2	2.55	0.41
1:B:228:ILE:O	1:B:229:ASP:OD1	2.38	0.41
1:A:256:SER:CA	1:A:310:HIS:HD2	2.33	0.41
1:B:271:GLY:O	1:B:273:LEU:N	2.54	0.41
1:B:256:SER:C	1:B:258:HIS:N	2.70	0.41
1:A:118:ILE:HG12	1:B:25:LEU:HB2	2.03	0.41
1:A:236:SER:C	1:A:237:VAL:CG1	2.90	0.41
1:A:257:SER:O	1:A:311:TRP:HB3	2.21	0.41
1:B:29:PRO:O	1:B:205:GLY:HA3	2.21	0.41
1:B:250:ILE:HD12	1:B:313:LEU:CD2	2.32	0.41
1:B:250:ILE:HG21	1:B:270:LEU:CD1	2.51	0.41
1:A:133:HIS:ND1	1:A:184:HIS:HB2	2.35	0.41
1:A:27:LYS:O	1:B:116:ARG:HD2	2.21	0.41
1:A:153:LYS:NZ	5:A:838:HOH:O	2.54	0.41
1:B:207:LYS:HB2	1:B:308:TYR:CE2	2.56	0.41
1:A:306:LEU:HB2	1:A:307:PRO:HD3	2.03	0.41
1:A:37:PHE:HA	1:A:334:ASN:O	2.21	0.41
1:A:44:ARG:HE	1:A:47:ASP:CG	2.25	0.41
1:B:226:PHE:CB	1:B:342:ALA:HB2	2.50	0.41
1:B:226:PHE:CE2	1:B:339:GLU:HG3	2.55	0.41
1:A:25:LEU:HB2	1:B:118:ILE:HG13	2.02	0.41
1:B:225:HIS:HB3	1:B:238:ALA:O	2.20	0.41
1:B:118:ILE:O	1:B:119:VAL:C	2.58	0.41
1:A:230:GLU:HG3	1:A:234:PHE:O	2.21	0.41
1:A:155:ARG:O	1:A:156:ILE:C	2.59	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:226:PHE:HB3	1:B:342:ALA:CB	2.50	0.41
1:B:341:VAL:HG21	4:B:610:EDO:H22	2.03	0.41
1:B:320:SER:HA	5:B:778:HOH:O	2.20	0.41
1:A:270:LEU:C	1:A:272:GLY:N	2.73	0.41
1:A:324:GLY:CA	1:B:293:MET:HE1	2.51	0.41
1:B:95:LEU:C	1:B:97:PRO:HD3	2.41	0.41
1:B:184:HIS:O	1:B:185:SER:C	2.59	0.41
1:A:234:PHE:CE2	1:A:252:PRO:HB3	2.55	0.41
1:A:325:PHE:HB3	5:A:679:HOH:O	2.20	0.41
1:B:270:LEU:O	1:B:271:GLY:O	2.39	0.41
1:A:94:ASN:ND2	1:A:124:HIS:CE1	2.89	0.41
1:A:166:ASN:CG	1:A:300:LYS:HZ1	2.24	0.41
1:B:101:ARG:HH12	1:B:124:HIS:N	2.15	0.41
1:B:70:GLU:C	1:B:72:GLU:H	2.23	0.41
1:B:207:LYS:HD3	1:B:308:TYR:OH	2.21	0.41
1:B:186:HIS:CD2	1:B:186:HIS:N	2.87	0.41
1:A:188:GLN:OE1	3:A:601:AMP:H4'	2.21	0.41
1:A:214:GLY:O	1:A:215:LYS:HB3	2.20	0.41
1:A:44:ARG:HG2	1:A:46:THR:HG22	2.02	0.41
1:B:50:SER:HB2	1:B:288:PRO:HA	2.03	0.41
1:A:329:THR:HG22	1:B:196:PRO:HG3	2.03	0.41
1:B:63:CYS:HB2	1:B:64:PRO:HD2	2.03	0.41
1:B:171:PHE:HB2	1:B:292:TYR:O	2.21	0.41
1:A:281:ILE:CG2	1:A:285:LEU:HD12	2.50	0.41
1:A:120:GLY:HA2	1:B:25:LEU:HD23	2.02	0.41
1:A:140:ILE:HG23	1:A:144:GLY:HA3	2.03	0.40
1:A:254:ASP:CG	5:A:860:HOH:O	2.60	0.40
1:B:66:CYS:SG	1:B:133:HIS:HB2	2.61	0.40
1:A:218:LEU:HA	1:A:218:LEU:HD23	1.74	0.40
1:A:299:LEU:HD23	1:A:299:LEU:HA	1.87	0.40
1:A:28:ASP:HB3	1:A:31:THR:CG2	2.51	0.40
1:B:135:ILE:O	1:B:185:SER:HB2	2.20	0.40
1:A:138:SER:O	1:A:275:LYS:NZ	2.44	0.40
1:A:297:SER:OG	1:A:301:VAL:HB	2.20	0.40
1:B:290:TYR:HE2	1:B:292:TYR:CD2	2.38	0.40
1:B:156:ILE:HG23	1:B:168:ILE:HD12	2.03	0.40
1:A:94:ASN:O	1:A:97:PRO:HD3	2.21	0.40
1:B:93:GLU:HG2	1:B:101:ARG:HH22	1.87	0.40
1:B:33:ARG:HD3	5:B:711:HOH:O	2.19	0.40
1:A:156:ILE:CG1	1:A:189:MET:HE1	2.52	0.40
1:B:203:LEU:HD11	1:B:298:PRO:HG2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:137:LEU:HA	1:A:140:ILE:HD12	2.03	0.40
1:A:188:GLN:CD	3:A:601:AMP:H5'2	2.40	0.40
1:B:21:GLN:HG2	1:B:22:SER:N	2.27	0.40
1:B:50:SER:HB2	1:B:288:PRO:CB	2.50	0.40
1:A:44:ARG:O	1:A:47:ASP:HB2	2.21	0.40
1:A:182:MET:HB2	1:A:186:HIS:CD2	2.56	0.40
1:B:255:HIS:NE2	1:B:307:PRO:O	2.54	0.40
1:B:197:PRO:O	1:B:201:SER:HB2	2.21	0.40
1:B:195:VAL:CG1	1:B:199:VAL:HB	2.51	0.40
1:B:306:LEU:N	1:B:307:PRO:CD	2.85	0.40
1:A:173:ASN:HA	1:A:291:ASN:HD22	1.82	0.40
1:B:172:LYS:HG3	1:B:186:HIS:O	2.21	0.40
1:B:162:HIS:C	1:B:164:SER:H	2.25	0.40
1:A:219:CYS:CA	1:A:310:HIS:CE1	3.04	0.40
1:A:103:LEU:HD13	1:A:119:VAL:HB	2.02	0.40
1:A:82:ASP:O	1:A:84:ASP:N	2.54	0.40
1:A:225:HIS:HB3	1:A:238:ALA:O	2.21	0.40
1:A:239:PRO:HG3	1:A:249:TRP:CG	2.56	0.40
1:B:33:ARG:NH1	1:B:33:ARG:CG	2.84	0.40
1:A:297:SER:HA	1:A:298:PRO:HD3	1.93	0.40
1:A:256:SER:O	1:A:310:HIS:HA	2.21	0.40
1:A:172:LYS:HB2	1:A:187:SER:OG	2.21	0.40
1:B:172:LYS:O	1:B:291:ASN:HA	2.20	0.40
1:A:252:PRO:HG3	1:A:311:TRP:CE2	2.56	0.40
1:A:51:LYS:HE2	1:A:319:LEU:O	2.21	0.40
1:A:346:ARG:HD3	5:A:881:HOH:O	2.22	0.40
1:A:89:LEU:HA	1:A:128:ILE:O	2.22	0.40
1:B:236:SER:HA	1:B:249:TRP:O	2.20	0.40
1:B:67:ILE:HD12	1:B:70:GLU:OE2	2.21	0.40
1:B:165:ILE:CG2	1:B:166:ASN:H	2.35	0.40
1:A:282:ALA:HB1	1:A:287:ASP:OD1	2.21	0.40
1:B:103:LEU:HB3	1:B:106:GLN:NE2	2.36	0.40
1:B:335:PRO:O	1:B:336:VAL:CG2	2.69	0.40
1:B:343:LYS:O	1:B:347:GLU:HG2	2.21	0.40
1:B:197:PRO:O	1:B:200:SER:HB3	2.22	0.40
1:B:171:PHE:CE2	1:B:190:MET:HB2	2.56	0.40
1:A:233:HIS:C	1:A:234:PHE:CD1	2.94	0.40
1:B:141:ASP:CA	5:B:827:HOH:O	2.68	0.40
1:A:226:PHE:HB3	1:A:342:ALA:CB	2.51	0.40
1:B:71:GLN:HB2	5:B:716:HOH:O	2.20	0.40
1:B:220:GLU:O	1:B:224:LYS:HG2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:324:GLY:HA3	1:B:171:PHE:CD1	2.56	0.40
1:B:244:TYR:O	1:B:247:GLU:HB2	2.21	0.40
1:B:171:PHE:HA	1:B:292:TYR:O	2.21	0.40
1:B:172:LYS:HD3	1:B:290:TYR:CE2	2.56	0.40
1:B:259:PHE:HD1	1:B:311:TRP:CZ3	2.39	0.40
1:B:185:SER:O	1:B:186:HIS:HB3	2.21	0.40
1:B:318:GLN:HG2	4:B:612:EDO:O2	2.21	0.40
1:B:129:GLU:CD	1:B:137:LEU:HD12	2.41	0.40
1:B:345:MET:HA	1:B:348:VAL:HG23	2.03	0.40
1:A:128:ILE:HA	1:A:186:HIS:HB3	2.03	0.40
1:B:242:ALA:CB	4:B:610:EDO:H11	2.51	0.40
1:B:162:HIS:HB3	1:B:164:SER:OG	2.22	0.40
1:A:117:THR:HG22	1:A:118:ILE:N	2.35	0.40
1:A:226:PHE:HD2	1:A:338:PRO:HB2	1.85	0.40
1:A:63:CYS:SG	1:A:184:HIS:HB2	2.62	0.40
1:B:252:PRO:HG2	1:B:310:HIS:HE2	1.87	0.40
1:B:172:LYS:HB3	1:B:292:TYR:CB	2.24	0.40
1:B:247:GLU:HG2	1:B:248:ILE:N	2.36	0.40
1:B:226:PHE:CZ	1:B:339:GLU:HG3	2.57	0.40
1:A:202:ARG:O	1:A:203:LEU:C	2.59	0.40
1:A:64:PRO:HG3	1:A:72:GLU:OE1	2.22	0.40
1:A:44:ARG:O	1:A:46:THR:N	2.55	0.40
1:A:234:PHE:CD2	1:A:252:PRO:HA	2.57	0.40
1:A:252:PRO:O	1:A:310:HIS:HE1	2.05	0.40
1:A:243:THR:HG23	1:A:332:TYR:CD2	2.57	0.40
1:B:172:LYS:HG2	1:B:290:TYR:CE2	2.56	0.40
1:B:277:MET:HA	1:B:277:MET:HE2	2.04	0.40
1:A:118:ILE:HG13	1:B:25:LEU:CB	2.48	0.40
1:B:244:TYR:O	1:B:334:ASN:ND2	2.54	0.40
1:B:181:SER:N	3:B:602:AMP:O2P	2.54	0.40
1:B:63:CYS:HB2	1:B:64:PRO:CD	2.52	0.40
1:A:172:LYS:HB3	1:A:292:TYR:CD1	2.57	0.40
1:A:188:GLN:NE2	3:A:601:AMP:O1P	2.54	0.40
1:B:297:SER:OG	1:B:298:PRO:N	2.54	0.40
1:B:66:CYS:HA	1:B:184:HIS:CE1	2.56	0.40
1:A:28:ASP:CG	1:A:29:PRO:HD2	2.41	0.40
1:B:177:SER:OG	1:B:289:PRO:HG2	2.21	0.40
1:B:141:ASP:HA	5:B:829:HOH:O	2.21	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1-A	303/351 (86%)	275 (91%)	25 (8%)	3 (1%)	19	6
1	1-B	297/351 (85%)	270 (91%)	22 (7%)	5 (2%)	11	2
1	2-A	303/351 (86%)	279 (92%)	20 (7%)	4 (1%)	15	4
1	2-B	297/351 (85%)	276 (93%)	18 (6%)	3 (1%)	19	6
1	3-A	303/351 (86%)	282 (93%)	18 (6%)	3 (1%)	19	6
1	3-B	297/351 (85%)	271 (91%)	22 (7%)	4 (1%)	15	4
1	4-A	303/351 (86%)	279 (92%)	20 (7%)	4 (1%)	15	4
1	4-B	297/351 (85%)	266 (90%)	27 (9%)	4 (1%)	15	4
1	5-A	303/351 (86%)	275 (91%)	22 (7%)	6 (2%)	9	1
1	5-B	297/351 (85%)	267 (90%)	26 (9%)	4 (1%)	15	4
1	6-A	303/351 (86%)	268 (88%)	27 (9%)	8 (3%)	7	0
1	6-B	297/351 (85%)	267 (90%)	28 (9%)	2 (1%)	26	10
1	7-A	303/351 (86%)	273 (90%)	25 (8%)	5 (2%)	11	2
1	7-B	297/351 (85%)	276 (93%)	18 (6%)	3 (1%)	19	6
1	8-A	303/351 (86%)	290 (96%)	10 (3%)	3 (1%)	19	6
1	8-B	297/351 (85%)	266 (90%)	27 (9%)	4 (1%)	15	4
All	All	4800/5616 (86%)	4380 (91%)	355 (7%)	65 (1%)	14	3

All (65) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1-B	320	SER
1	2-A	30	VAL
1	3-A	75	PRO
1	3-A	220	GLU
1	3-B	30	VAL
1	3-B	83	HIS

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Mol	Chain	Res	Type
1	4-A	242	ALA
1	4-B	85	PRO
1	5-A	84	ASP
1	6-A	320	SER
1	8-A	83	HIS
1	8-B	197	PRO
1	8-B	262	LEU
1	1-A	29	PRO
1	1-B	49	LYS
1	1-B	232	SER
1	2-A	185	SER
1	2-B	327	ILE
1	3-B	348	VAL
1	4-A	347	GLU
1	4-B	271	GLY
1	4-B	272	GLY
1	5-A	82	ASP
1	5-B	32	ASN
1	5-B	47	ASP
1	7-A	164	SER
1	7-B	120	GLY
1	8-A	98	ALA
1	1-A	260	HIS
1	2-A	83	HIS
1	2-A	260	HIS
1	4-B	328	GLY
1	5-A	119	VAL
1	5-A	240	PHE
1	5-B	336	VAL
1	6-A	51	LYS
1	6-A	154	LYS
1	6-A	161	GLN
1	6-A	277	MET
1	6-A	283	LYS
1	7-B	83	HIS
1	8-A	102	ASN
1	4-A	212	GLU
1	4-A	307	PRO
1	5-A	83	HIS
1	5-B	33	ARG
1	6-A	278	LEU
1	7-A	50	SER

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Mol	Chain	Res	Type
1	7-A	202	ARG
1	1-B	257	SER
1	2-B	22	SER
1	2-B	333	ILE
1	3-A	83	HIS
1	3-B	253	LYS
1	6-A	235	VAL
1	6-B	68	GLY
1	8-B	203	LEU
1	8-B	240	PHE
1	7-A	45	PRO
1	7-A	260	HIS
1	7-B	69	ARG
1	6-B	67	ILE
1	1-A	45	PRO
1	1-B	131	PRO
1	5-A	237	VAL

### 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-A	280/312 (90%)	277 (99%)	3 (1%)	80	72
1	1-B	274/312 (88%)	264 (96%)	10 (4%)	42	21
1	2-A	280/312 (90%)	274 (98%)	6 (2%)	61	45
1	2-B	274/312 (88%)	264 (96%)	10 (4%)	42	21
1	3-A	280/312 (90%)	271 (97%)	9 (3%)	46	26
1	3-B	274/312 (88%)	264 (96%)	10 (4%)	42	21
1	4-A	280/312 (90%)	275 (98%)	5 (2%)	66	52
1	4-B	274/312 (88%)	273 (100%)	1 (0%)	93	92
1	5-A	280/312 (90%)	272 (97%)	8 (3%)	50	30
1	5-B	274/312 (88%)	262 (96%)	12 (4%)	35	15
1	6-A	280/312 (90%)	273 (98%)	7 (2%)	55	37

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	6-B	274/312 (88%)	264 (96%)	10 (4%)	42	21
1	7-A	280/312 (90%)	267 (95%)	13 (5%)	33	13
1	7-B	274/312 (88%)	268 (98%)	6 (2%)	60	43
1	8-A	280/312 (90%)	274 (98%)	6 (2%)	61	45
1	8-B	274/312 (88%)	270 (98%)	4 (2%)	72	60
All	All	4432/4992 (89%)	4312 (97%)	120 (3%)	52	34

All (120) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1-A	33	ARG
1	1-A	78	PHE
1	1-A	258	HIS
1	1-B	21	GLN
1	1-B	101	ARG
1	1-B	134	SER
1	1-B	139	ASP
1	1-B	141	ASP
1	1-B	260	HIS
1	1-B	261	HIS
1	1-B	288	PRO
1	1-B	289	PRO
1	1-B	318	GLN
1	2-A	31	THR
1	2-A	60	PRO
1	2-A	189	MET
1	2-A	216	CYS
1	2-A	292	TYR
1	2-A	293	MET
1	2-B	25	LEU
1	2-B	33	ARG
1	2-B	63	CYS
1	2-B	71	GLN
1	2-B	101	ARG
1	2-B	163	ASP
1	2-B	182	MET
1	2-B	200	SER
1	2-B	292	TYR
1	2-B	332	TYR
1	3-A	22	SER

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Mol	Chain	Res	Type
1	3-A	60	PRO
1	3-A	117	THR
1	3-A	141	ASP
1	3-A	187	SER
1	3-A	266	LYS
1	3-A	279	GLN
1	3-A	292	TYR
1	3-A	293	MET
1	3-B	25	LEU
1	3-B	39	PRO
1	3-B	46	THR
1	3-B	63	CYS
1	3-B	67	ILE
1	3-B	163	ASP
1	3-B	186	HIS
1	3-B	219	CYS
1	3-B	264	ASP
1	3-B	349	SER
1	4-A	116	ARG
1	4-A	186	HIS
1	4-A	219	CYS
1	4-A	264	ASP
1	4-A	292	TYR
1	4-B	292	TYR
1	5-A	33	ARG
1	5-A	63	CYS
1	5-A	187	SER
1	5-A	219	CYS
1	5-A	251	ILE
1	5-A	292	TYR
1	5-A	310	HIS
1	5-A	334	ASN
1	5-B	22	SER
1	5-B	38	SER
1	5-B	47	ASP
1	5-B	69	ARG
1	5-B	71	GLN
1	5-B	164	SER
1	5-B	194	VAL
1	5-B	258	HIS
1	5-B	262	LEU
1	5-B	292	TYR

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Mol	Chain	Res	Type
1	5-B	297	SER
1	5-B	304	SER
1	6-A	52	SER
1	6-A	117	THR
1	6-A	174	GLN
1	6-A	275	LYS
1	6-A	277	MET
1	6-A	318	GLN
1	6-A	340	ASP
1	6-B	22	SER
1	6-B	25	LEU
1	6-B	28	ASP
1	6-B	38	SER
1	6-B	46	THR
1	6-B	101	ARG
1	6-B	135	ILE
1	6-B	187	SER
1	6-B	258	HIS
1	6-B	309	THR
1	7-A	31	THR
1	7-A	46	THR
1	7-A	116	ARG
1	7-A	125	ASP
1	7-A	141	ASP
1	7-A	171	PHE
1	7-A	185	SER
1	7-A	186	HIS
1	7-A	212	GLU
1	7-A	219	CYS
1	7-A	224	LYS
1	7-A	293	MET
1	7-A	334	ASN
1	7-B	47	ASP
1	7-B	63	CYS
1	7-B	292	TYR
1	7-B	293	MET
1	7-B	297	SER
1	7-B	336	VAL
1	8-A	25	LEU
1	8-A	86	ASN
1	8-A	187	SER
1	8-A	192	LEU

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Mol	Chain	Res	Type
1	8-A	297	SER
1	8-A	332	TYR
1	8-B	22	SER
1	8-B	67	ILE
1	8-B	101	ARG
1	8-B	217	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (78) such sidechains are listed below:

Mol	Chain	Res	Type
1	1-A	86	ASN
1	1-A	286	ASN
1	1-B	106	GLN
1	1-B	233	HIS
1	1-B	286	ASN
1	1-B	291	ASN
1	1-B	318	GLN
1	2-A	94	ASN
1	2-A	158	GLN
1	2-A	261	HIS
1	2-A	318	GLN
1	2-B	106	GLN
1	2-B	136	GLN
1	2-B	161	GLN
1	2-B	186	HIS
1	2-B	291	ASN
1	2-B	318	GLN
1	3-A	86	ASN
1	3-A	162	HIS
1	3-A	169	GLN
1	3-A	260	HIS
1	3-B	21	GLN
1	3-B	71	GLN
1	3-B	136	GLN
1	3-B	284	GLN
1	3-B	286	ASN
1	3-B	318	GLN
1	4-A	169	GLN
1	4-A	186	HIS
1	4-A	261	HIS
1	4-A	286	ASN
1	4-A	310	HIS

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Mol	Chain	Res	Type
1	4-B	32	ASN
1	4-B	83	HIS
1	4-B	106	GLN
1	4-B	157	ASN
1	4-B	173	ASN
1	4-B	258	HIS
1	4-B	260	HIS
1	4-B	286	ASN
1	4-B	291	ASN
1	5-A	71	GLN
1	5-A	86	ASN
1	5-A	260	HIS
1	5-A	334	ASN
1	5-B	83	HIS
1	5-B	106	GLN
1	5-B	161	GLN
1	5-B	233	HIS
1	5-B	258	HIS
1	5-B	291	ASN
1	6-A	86	ASN
1	6-A	166	ASN
1	6-A	174	GLN
1	6-B	21	GLN
1	6-B	83	HIS
1	6-B	136	GLN
1	6-B	161	GLN
1	6-B	233	HIS
1	6-B	258	HIS
1	6-B	260	HIS
1	7-A	318	GLN
1	7-A	334	ASN
1	7-B	21	GLN
1	7-B	83	HIS
1	7-B	136	GLN
1	7-B	161	GLN
1	7-B	258	HIS
1	7-B	260	HIS
1	8-A	86	ASN
1	8-A	260	HIS
1	8-B	106	GLN
1	8-B	136	GLN
1	8-B	161	GLN

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Mol	Chain	Res	Type
1	8-B	258	HIS
1	8-B	261	HIS
1	8-B	295	HIS
1	8-B	314	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 5.6 Ligand geometry ⓘ

Of 96 ligands modelled in this entry, 32 are monoatomic - leaving 64 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	AMP	1-A	601	-	15,24,25	2.07	4 (26%)	16,35,38	3.26	3 (18%)
4	EDO	1-A	607	-	3,3,3	0.52	0	2,2,2	0.36	0
4	EDO	1-A	608	-	3,3,3	0.63	0	2,2,2	0.55	0
4	EDO	1-A	609	-	3,3,3	0.34	0	2,2,2	0.55	0
3	AMP	1-B	602	-	15,24,25	1.60	3 (20%)	16,35,38	3.39	4 (25%)
4	EDO	1-B	610	-	3,3,3	0.54	0	2,2,2	0.37	0
4	EDO	1-B	611	-	3,3,3	0.59	0	2,2,2	0.42	0
4	EDO	1-B	612	-	3,3,3	0.29	0	2,2,2	0.52	0
3	AMP	2-A	601	-	15,24,25	2.11	4 (26%)	16,35,38	3.31	4 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	EDO	2-A	607	-	3,3,3	0.45	0	2,2,2	0.43	0
4	EDO	2-A	608	-	3,3,3	0.59	0	2,2,2	0.57	0
4	EDO	2-A	609	-	3,3,3	0.32	0	2,2,2	0.54	0
3	AMP	2-B	602	-	15,24,25	1.65	4 (26%)	16,35,38	3.56	5 (31%)
4	EDO	2-B	610	-	3,3,3	0.62	0	2,2,2	0.41	0
4	EDO	2-B	611	-	3,3,3	0.59	0	2,2,2	0.41	0
4	EDO	2-B	612	-	3,3,3	0.29	0	2,2,2	0.54	0
3	AMP	3-A	601	-	15,24,25	2.03	4 (26%)	16,35,38	3.21	2 (12%)
4	EDO	3-A	607	-	3,3,3	0.50	0	2,2,2	0.54	0
4	EDO	3-A	608	-	3,3,3	0.62	0	2,2,2	0.50	0
4	EDO	3-A	609	-	3,3,3	0.33	0	2,2,2	0.52	0
3	AMP	3-B	602	-	15,24,25	1.64	4 (26%)	16,35,38	3.40	5 (31%)
4	EDO	3-B	610	-	3,3,3	0.62	0	2,2,2	0.25	0
4	EDO	3-B	611	-	3,3,3	0.60	0	2,2,2	0.40	0
4	EDO	3-B	612	-	3,3,3	0.28	0	2,2,2	0.52	0
3	AMP	4-A	601	-	15,24,25	2.00	4 (26%)	16,35,38	3.15	3 (18%)
4	EDO	4-A	607	-	3,3,3	0.56	0	2,2,2	0.44	0
4	EDO	4-A	608	-	3,3,3	0.62	0	2,2,2	0.54	0
4	EDO	4-A	609	-	3,3,3	0.39	0	2,2,2	0.55	0
3	AMP	4-B	602	-	15,24,25	1.86	4 (26%)	16,35,38	3.60	5 (31%)
4	EDO	4-B	610	-	3,3,3	0.70	0	2,2,2	0.17	0
4	EDO	4-B	611	-	3,3,3	0.57	0	2,2,2	0.37	0
4	EDO	4-B	612	-	3,3,3	0.29	0	2,2,2	0.55	0
3	AMP	5-A	601	-	15,24,25	2.21	5 (33%)	16,35,38	3.84	6 (37%)
4	EDO	5-A	607	-	3,3,3	0.62	0	2,2,2	0.24	0
4	EDO	5-A	608	-	3,3,3	0.65	0	2,2,2	0.42	0
4	EDO	5-A	609	-	3,3,3	0.34	0	2,2,2	0.56	0
3	AMP	5-B	602	-	15,24,25	1.74	4 (26%)	16,35,38	3.73	6 (37%)
4	EDO	5-B	610	-	3,3,3	0.54	0	2,2,2	0.36	0
4	EDO	5-B	611	-	3,3,3	0.68	0	2,2,2	0.36	0
4	EDO	5-B	612	-	3,3,3	0.27	0	2,2,2	0.58	0
3	AMP	6-A	601	-	15,24,25	2.10	4 (26%)	16,35,38	3.70	6 (37%)
4	EDO	6-A	607	-	3,3,3	0.52	0	2,2,2	0.34	0
4	EDO	6-A	608	-	3,3,3	0.63	0	2,2,2	0.51	0
4	EDO	6-A	609	-	3,3,3	0.39	0	2,2,2	0.60	0
3	AMP	6-B	602	-	15,24,25	1.68	4 (26%)	16,35,38	3.69	7 (43%)
4	EDO	6-B	610	-	3,3,3	0.69	0	2,2,2	0.25	0
4	EDO	6-B	611	-	3,3,3	0.62	0	2,2,2	0.36	0
4	EDO	6-B	612	-	3,3,3	0.91	0	2,2,2	0.38	0
3	AMP	7-A	601	-	15,24,25	2.11	4 (26%)	16,35,38	3.63	5 (31%)
4	EDO	7-A	607	-	3,3,3	0.49	0	2,2,2	0.45	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	EDO	7-A	608	-	3,3,3	0.62	0	2,2,2	0.48	0
4	EDO	7-A	609	-	3,3,3	0.71	0	2,2,2	0.27	0
3	AMP	7-B	602	-	15,24,25	1.91	3 (20%)	16,35,38	3.79	5 (31%)
4	EDO	7-B	610	-	3,3,3	0.68	0	2,2,2	0.32	0
4	EDO	7-B	611	-	3,3,3	0.61	0	2,2,2	0.40	0
4	EDO	7-B	612	-	3,3,3	0.31	0	2,2,2	0.63	0
3	AMP	8-A	601	-	15,24,25	2.08	4 (26%)	16,35,38	3.71	5 (31%)
4	EDO	8-A	607	-	3,3,3	0.54	0	2,2,2	0.41	0
4	EDO	8-A	608	-	3,3,3	0.63	0	2,2,2	0.56	0
4	EDO	8-A	609	-	3,3,3	0.39	0	2,2,2	0.52	0
3	AMP	8-B	602	-	15,24,25	1.50	3 (20%)	16,35,38	3.60	6 (37%)
4	EDO	8-B	610	-	3,3,3	0.72	0	2,2,2	0.17	0
4	EDO	8-B	611	-	3,3,3	0.60	0	2,2,2	0.41	0
4	EDO	8-B	612	-	3,3,3	0.25	0	2,2,2	0.57	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	AMP	1-A	601	-	-	0/3/25/26	0/3/3/3
4	EDO	1-A	607	-	-	0/1/1/1	0/0/0/0
4	EDO	1-A	608	-	-	0/1/1/1	0/0/0/0
4	EDO	1-A	609	-	-	0/1/1/1	0/0/0/0
3	AMP	1-B	602	-	-	0/3/25/26	0/3/3/3
4	EDO	1-B	610	-	-	0/1/1/1	0/0/0/0
4	EDO	1-B	611	-	-	0/1/1/1	0/0/0/0
4	EDO	1-B	612	-	-	0/1/1/1	0/0/0/0
3	AMP	2-A	601	-	-	0/3/25/26	0/3/3/3
4	EDO	2-A	607	-	-	0/1/1/1	0/0/0/0
4	EDO	2-A	608	-	-	0/1/1/1	0/0/0/0
4	EDO	2-A	609	-	-	0/1/1/1	0/0/0/0
3	AMP	2-B	602	-	-	0/3/25/26	0/3/3/3
4	EDO	2-B	610	-	-	0/1/1/1	0/0/0/0
4	EDO	2-B	611	-	-	0/1/1/1	0/0/0/0
4	EDO	2-B	612	-	-	0/1/1/1	0/0/0/0
3	AMP	3-A	601	-	-	0/3/25/26	0/3/3/3
4	EDO	3-A	607	-	-	0/1/1/1	0/0/0/0
4	EDO	3-A	608	-	-	0/1/1/1	0/0/0/0
4	EDO	3-A	609	-	-	0/1/1/1	0/0/0/0
3	AMP	3-B	602	-	-	0/3/25/26	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	3-B	610	-	-	0/1/1/1	0/0/0/0
4	EDO	3-B	611	-	-	0/1/1/1	0/0/0/0
4	EDO	3-B	612	-	-	0/1/1/1	0/0/0/0
3	AMP	4-A	601	-	-	0/3/25/26	0/3/3/3
4	EDO	4-A	607	-	-	0/1/1/1	0/0/0/0
4	EDO	4-A	608	-	-	0/1/1/1	0/0/0/0
4	EDO	4-A	609	-	-	0/1/1/1	0/0/0/0
3	AMP	4-B	602	-	-	0/3/25/26	0/3/3/3
4	EDO	4-B	610	-	-	0/1/1/1	0/0/0/0
4	EDO	4-B	611	-	-	0/1/1/1	0/0/0/0
4	EDO	4-B	612	-	-	0/1/1/1	0/0/0/0
3	AMP	5-A	601	-	-	0/3/25/26	0/3/3/3
4	EDO	5-A	607	-	-	0/1/1/1	0/0/0/0
4	EDO	5-A	608	-	-	0/1/1/1	0/0/0/0
4	EDO	5-A	609	-	-	0/1/1/1	0/0/0/0
3	AMP	5-B	602	-	-	0/3/25/26	0/3/3/3
4	EDO	5-B	610	-	-	0/1/1/1	0/0/0/0
4	EDO	5-B	611	-	-	0/1/1/1	0/0/0/0
4	EDO	5-B	612	-	-	0/1/1/1	0/0/0/0
3	AMP	6-A	601	-	-	0/3/25/26	0/3/3/3
4	EDO	6-A	607	-	-	0/1/1/1	0/0/0/0
4	EDO	6-A	608	-	-	0/1/1/1	0/0/0/0
4	EDO	6-A	609	-	-	0/1/1/1	0/0/0/0
3	AMP	6-B	602	-	-	0/3/25/26	0/3/3/3
4	EDO	6-B	610	-	-	0/1/1/1	0/0/0/0
4	EDO	6-B	611	-	-	0/1/1/1	0/0/0/0
4	EDO	6-B	612	-	-	0/1/1/1	0/0/0/0
3	AMP	7-A	601	-	-	0/3/25/26	0/3/3/3
4	EDO	7-A	607	-	-	0/1/1/1	0/0/0/0
4	EDO	7-A	608	-	-	0/1/1/1	0/0/0/0
4	EDO	7-A	609	-	-	0/1/1/1	0/0/0/0
3	AMP	7-B	602	-	-	0/3/25/26	0/3/3/3
4	EDO	7-B	610	-	-	0/1/1/1	0/0/0/0
4	EDO	7-B	611	-	-	0/1/1/1	0/0/0/0
4	EDO	7-B	612	-	-	0/1/1/1	0/0/0/0
3	AMP	8-A	601	-	-	0/3/25/26	0/3/3/3
4	EDO	8-A	607	-	-	0/1/1/1	0/0/0/0
4	EDO	8-A	608	-	-	0/1/1/1	0/0/0/0
4	EDO	8-A	609	-	-	0/1/1/1	0/0/0/0
3	AMP	8-B	602	-	-	0/3/25/26	0/3/3/3
4	EDO	8-B	610	-	-	0/1/1/1	0/0/0/0
4	EDO	8-B	611	-	-	0/1/1/1	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	8-B	612	-	-	0/1/1/1	0/0/0/0

All (62) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	4-B	602	AMP	O4'-C1'	-2.84	1.37	1.41
3	4-A	601	AMP	O3'-C3'	-2.27	1.37	1.43
3	2-B	602	AMP	O4'-C1'	-2.15	1.38	1.41
3	3-B	602	AMP	O4'-C1'	-2.05	1.38	1.41
3	6-B	602	AMP	C8-N7	2.08	1.38	1.34
3	1-B	602	AMP	C4-N3	2.09	1.38	1.35
3	5-B	602	AMP	C8-N7	2.10	1.38	1.34
3	5-A	601	AMP	C5'-C4'	2.13	1.58	1.51
3	3-B	602	AMP	C4-N3	2.19	1.38	1.35
3	5-B	602	AMP	C4-N3	2.24	1.38	1.35
3	8-B	602	AMP	C4-N3	2.24	1.38	1.35
3	2-B	602	AMP	C4-N3	2.29	1.39	1.35
3	6-B	602	AMP	C4-N3	2.38	1.39	1.35
3	3-A	601	AMP	O4'-C1'	2.44	1.44	1.41
3	4-B	602	AMP	C4-N3	2.49	1.39	1.35
3	8-A	601	AMP	O4'-C1'	2.52	1.44	1.41
3	3-A	601	AMP	C4-N3	2.54	1.39	1.35
3	4-A	601	AMP	C4-N3	2.63	1.39	1.35
3	7-B	602	AMP	C4-N3	2.65	1.39	1.35
3	8-B	602	AMP	C2-N1	2.72	1.39	1.33
3	1-A	601	AMP	C4-N3	2.77	1.39	1.35
3	6-A	601	AMP	O4'-C1'	2.79	1.44	1.41
3	5-A	601	AMP	C4-N3	2.88	1.39	1.35
3	7-A	601	AMP	O4'-C1'	2.89	1.44	1.41
3	2-A	601	AMP	C4-N3	2.91	1.39	1.35
3	7-A	601	AMP	C4-N3	2.91	1.39	1.35
3	3-B	602	AMP	C2-N1	2.94	1.39	1.33
3	6-A	601	AMP	C4-N3	2.98	1.40	1.35
3	6-B	602	AMP	C2-N1	3.06	1.39	1.33
3	5-A	601	AMP	O4'-C1'	3.08	1.45	1.41
3	1-A	601	AMP	O4'-C1'	3.11	1.45	1.41
3	8-A	601	AMP	C4-N3	3.16	1.40	1.35
3	2-B	602	AMP	C2-N1	3.17	1.39	1.33
3	1-B	602	AMP	C2-N1	3.18	1.39	1.33
3	2-A	601	AMP	O4'-C1'	3.21	1.45	1.41
3	4-A	601	AMP	C2-N1	3.23	1.40	1.33
3	3-A	601	AMP	C2-N1	3.32	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	5-B	602	AMP	C2-N1	3.33	1.40	1.33
3	7-A	601	AMP	C2-N1	3.39	1.40	1.33
3	4-B	602	AMP	C2-N1	3.40	1.40	1.33
3	2-A	601	AMP	C2-N1	3.42	1.40	1.33
3	1-A	601	AMP	C2-N1	3.47	1.40	1.33
3	5-A	601	AMP	C2-N1	3.60	1.40	1.33
3	8-A	601	AMP	C2-N1	3.63	1.40	1.33
3	7-B	602	AMP	C2-N1	3.65	1.40	1.33
3	6-A	601	AMP	C2-N1	3.65	1.40	1.33
3	2-B	602	AMP	C2-N3	3.74	1.38	1.32
3	3-B	602	AMP	C2-N3	3.98	1.39	1.32
3	8-B	602	AMP	C2-N3	4.01	1.39	1.32
3	4-B	602	AMP	C2-N3	4.08	1.39	1.32
3	5-B	602	AMP	C2-N3	4.11	1.39	1.32
3	1-B	602	AMP	C2-N3	4.13	1.39	1.32
3	6-B	602	AMP	C2-N3	4.14	1.39	1.32
3	7-B	602	AMP	C2-N3	4.46	1.40	1.32
3	5-A	601	AMP	C2-N3	5.09	1.41	1.32
3	8-A	601	AMP	C2-N3	5.10	1.41	1.32
3	7-A	601	AMP	C2-N3	5.18	1.41	1.32
3	6-A	601	AMP	C2-N3	5.33	1.41	1.32
3	2-A	601	AMP	C2-N3	5.34	1.41	1.32
3	1-A	601	AMP	C2-N3	5.35	1.41	1.32
3	3-A	601	AMP	C2-N3	5.37	1.41	1.32
3	4-A	601	AMP	C2-N3	5.57	1.42	1.32

All (77) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	5-B	602	AMP	N3-C2-N1	-12.62	119.23	128.89
3	4-B	602	AMP	N3-C2-N1	-12.57	119.27	128.89
3	2-B	602	AMP	N3-C2-N1	-12.43	119.38	128.89
3	6-B	602	AMP	N3-C2-N1	-12.41	119.39	128.89
3	1-B	602	AMP	N3-C2-N1	-12.36	119.43	128.89
3	7-B	602	AMP	N3-C2-N1	-12.33	119.45	128.89
3	8-B	602	AMP	N3-C2-N1	-12.30	119.47	128.89
3	3-B	602	AMP	N3-C2-N1	-12.25	119.51	128.89
3	7-A	601	AMP	N3-C2-N1	-12.12	119.62	128.89
3	6-A	601	AMP	N3-C2-N1	-11.99	119.72	128.89
3	1-A	601	AMP	N3-C2-N1	-11.98	119.72	128.89
3	2-A	601	AMP	N3-C2-N1	-11.92	119.76	128.89
3	3-A	601	AMP	N3-C2-N1	-11.91	119.77	128.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	5-A	601	AMP	N3-C2-N1	-11.91	119.78	128.89
3	8-A	601	AMP	N3-C2-N1	-11.70	119.93	128.89
3	4-A	601	AMP	N3-C2-N1	-11.36	120.20	128.89
3	5-A	601	AMP	C4'-O4'-C1'	-4.67	104.58	109.72
3	8-A	601	AMP	C4'-O4'-C1'	-3.63	105.72	109.72
3	6-A	601	AMP	C4'-O4'-C1'	-3.52	105.86	109.72
3	2-B	602	AMP	C1'-N9-C4	-3.33	121.92	126.94
3	8-A	601	AMP	C1'-N9-C4	-3.31	121.95	126.94
3	5-A	601	AMP	C1'-N9-C4	-3.24	122.05	126.94
3	6-A	601	AMP	C1'-N9-C4	-3.11	122.25	126.94
3	4-B	602	AMP	C1'-N9-C4	-3.05	122.34	126.94
3	8-B	602	AMP	C1'-N9-C4	-2.89	122.58	126.94
3	7-A	601	AMP	C1'-N9-C4	-2.85	122.64	126.94
3	7-B	602	AMP	C1'-N9-C4	-2.82	122.68	126.94
3	5-B	602	AMP	C1'-N9-C4	-2.73	122.83	126.94
3	6-B	602	AMP	C1'-N9-C4	-2.55	123.09	126.94
3	7-A	601	AMP	C4'-O4'-C1'	-2.32	107.17	109.72
3	3-B	602	AMP	C1'-N9-C4	-2.21	123.61	126.94
3	2-A	601	AMP	C1'-N9-C4	-2.16	123.68	126.94
3	1-A	601	AMP	O4'-C4'-C5'	2.03	116.60	109.32
3	3-B	602	AMP	O4'-C1'-N9	2.09	112.47	108.10
3	5-B	602	AMP	C2-N1-C6	2.12	122.56	118.77
3	4-A	601	AMP	C2'-C1'-N9	2.15	117.57	114.29
3	8-B	602	AMP	O4'-C1'-N9	2.19	112.69	108.10
3	1-B	602	AMP	C2-N1-C6	2.21	122.72	118.77
3	6-B	602	AMP	C2-N1-C6	2.25	122.78	118.77
3	8-B	602	AMP	C2-N1-C6	2.25	122.79	118.77
3	1-B	602	AMP	C2'-C1'-N9	2.29	117.80	114.29
3	6-A	601	AMP	O5'-C5'-C4'	2.30	117.55	109.12
3	2-B	602	AMP	C2-N1-C6	2.35	122.96	118.77
3	6-B	602	AMP	O4'-C1'-N9	2.35	113.03	108.10
3	6-B	602	AMP	O5'-C5'-C4'	2.36	117.75	109.12
3	3-B	602	AMP	C2-N1-C6	2.38	123.03	118.77
3	4-B	602	AMP	C2-N1-C6	2.52	123.28	118.77
3	3-A	601	AMP	O4'-C4'-C5'	2.54	118.42	109.32
3	3-B	602	AMP	O4'-C4'-C5'	2.58	118.54	109.32
3	2-B	602	AMP	O4'-C4'-C5'	2.75	119.15	109.32
3	5-A	601	AMP	O4'-C1'-N9	2.78	113.91	108.10
3	2-A	601	AMP	O4'-C4'-C5'	2.79	119.29	109.32
3	4-B	602	AMP	C2'-C1'-N9	2.92	118.75	114.29
3	1-A	601	AMP	C2'-C1'-N9	2.93	118.77	114.29
3	8-B	602	AMP	C2'-C1'-N9	3.04	118.94	114.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	1-B	602	AMP	C4'-O4'-C1'	3.08	113.10	109.72
3	4-A	601	AMP	C4'-O4'-C1'	3.13	113.15	109.72
3	5-B	602	AMP	O5'-C5'-C4'	3.22	120.92	109.12
3	2-B	602	AMP	C2'-C1'-N9	3.33	119.38	114.29
3	2-A	601	AMP	C2'-C1'-N9	3.61	119.81	114.29
3	6-B	602	AMP	C2'-C1'-N9	3.61	119.81	114.29
3	5-B	602	AMP	C2'-C1'-N9	3.96	120.35	114.29
3	7-B	602	AMP	C2'-C1'-N9	4.07	120.50	114.29
3	8-B	602	AMP	O4'-C4'-C5'	4.07	123.89	109.32
3	5-B	602	AMP	O4'-C4'-C5'	4.11	124.02	109.32
3	4-B	602	AMP	C4'-O4'-C1'	4.12	114.25	109.72
3	5-A	601	AMP	C2'-C1'-N9	4.15	120.63	114.29
3	6-A	601	AMP	O4'-C4'-C5'	4.22	124.41	109.32
3	7-B	602	AMP	O5'-C5'-C4'	4.23	124.62	109.12
3	7-A	601	AMP	C2'-C1'-N9	4.26	120.80	114.29
3	6-A	601	AMP	C2'-C1'-N9	4.45	121.09	114.29
3	7-A	601	AMP	O4'-C4'-C5'	4.47	125.32	109.32
3	7-B	602	AMP	C4'-O4'-C1'	4.49	114.65	109.72
3	6-B	602	AMP	O4'-C4'-C5'	4.52	125.49	109.32
3	8-A	601	AMP	O4'-C4'-C5'	4.66	126.00	109.32
3	8-A	601	AMP	C2'-C1'-N9	4.92	121.80	114.29
3	5-A	601	AMP	O4'-C4'-C5'	5.23	128.03	109.32

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

42 monomers are involved in 126 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	1-A	601	AMP	7	0
3	1-B	602	AMP	6	0
4	1-B	612	EDO	1	0
3	2-A	601	AMP	7	0
4	2-A	607	EDO	1	0
3	2-B	602	AMP	5	0
3	3-A	601	AMP	4	0
4	3-A	607	EDO	3	0
3	3-B	602	AMP	6	0
4	3-B	610	EDO	4	0
4	3-B	611	EDO	1	0
3	4-A	601	AMP	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	4-A	608	EDO	1	0
4	4-A	609	EDO	2	0
3	4-B	602	AMP	5	0
4	4-B	610	EDO	1	0
4	4-B	611	EDO	1	0
3	5-A	601	AMP	4	0
4	5-A	607	EDO	1	0
4	5-A	608	EDO	1	0
3	5-B	602	AMP	3	0
4	5-B	610	EDO	2	0
4	5-B	611	EDO	2	0
4	5-B	612	EDO	1	0
3	6-A	601	AMP	6	0
4	6-A	607	EDO	1	0
4	6-A	609	EDO	1	0
3	6-B	602	AMP	7	0
4	6-B	610	EDO	2	0
4	6-B	612	EDO	1	0
3	7-A	601	AMP	4	0
4	7-A	607	EDO	1	0
4	7-A	609	EDO	2	0
3	7-B	602	AMP	5	0
4	7-B	610	EDO	3	0
4	7-B	612	EDO	1	0
3	8-A	601	AMP	5	0
4	8-A	607	EDO	4	0
4	8-A	609	EDO	1	0
3	8-B	602	AMP	4	0
4	8-B	610	EDO	2	0
4	8-B	612	EDO	2	0

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	1-A	311/351 (88%)	-0.61	6 (1%) 70 67	8, 16, 33, 50	311 (100%)
1	1-B	305/351 (86%)	-0.44	7 (2%) 64 61	9, 18, 35, 58	305 (100%)
1	2-A	311/351 (88%)	-0.61	6 (1%) 70 67	8, 16, 33, 50	311 (100%)
1	2-B	305/351 (86%)	-0.44	7 (2%) 64 61	9, 18, 35, 58	305 (100%)
1	3-A	311/351 (88%)	-0.61	6 (1%) 70 67	8, 16, 33, 50	311 (100%)
1	3-B	305/351 (86%)	-0.44	7 (2%) 64 61	9, 18, 35, 58	305 (100%)
1	4-A	311/351 (88%)	-0.61	6 (1%) 70 67	8, 16, 33, 50	311 (100%)
1	4-B	305/351 (86%)	-0.44	7 (2%) 64 61	9, 18, 35, 58	305 (100%)
1	5-A	311/351 (88%)	-0.61	6 (1%) 70 67	8, 16, 33, 50	311 (100%)
1	5-B	305/351 (86%)	-0.44	7 (2%) 64 61	9, 18, 35, 58	305 (100%)
1	6-A	311/351 (88%)	-0.61	6 (1%) 70 67	8, 16, 33, 50	311 (100%)
1	6-B	305/351 (86%)	-0.44	7 (2%) 64 61	9, 18, 35, 58	305 (100%)
1	7-A	311/351 (88%)	-0.61	6 (1%) 70 67	8, 16, 33, 50	311 (100%)
1	7-B	305/351 (86%)	-0.44	7 (2%) 64 61	9, 18, 35, 58	305 (100%)
1	8-A	311/351 (88%)	-0.61	6 (1%) 70 67	8, 16, 33, 50	311 (100%)
1	8-B	305/351 (86%)	-0.44	7 (2%) 64 61	9, 18, 35, 58	305 (100%)
All	All	4928/5616 (87%)	-0.53	104 (2%) 68 64	8, 17, 35, 58	4928 (100%)

All (104) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	1-B	67	ILE	4.9
1	2-B	67	ILE	4.9
1	3-B	67	ILE	4.9
1	4-B	67	ILE	4.9
1	5-B	67	ILE	4.9

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Mol	Chain	Res	Type	RSRZ
1	6-B	67	ILE	4.9
1	7-B	67	ILE	4.9
1	8-B	67	ILE	4.9
1	1-B	47	ASP	4.8
1	2-B	47	ASP	4.8
1	3-B	47	ASP	4.8
1	4-B	47	ASP	4.8
1	5-B	47	ASP	4.8
1	6-B	47	ASP	4.8
1	7-B	47	ASP	4.8
1	8-B	47	ASP	4.8
1	1-A	52	SER	4.4
1	2-A	52	SER	4.4
1	3-A	52	SER	4.4
1	4-A	52	SER	4.4
1	5-A	52	SER	4.4
1	6-A	52	SER	4.4
1	7-A	52	SER	4.4
1	8-A	52	SER	4.4
1	1-A	83	HIS	4.4
1	2-A	83	HIS	4.4
1	3-A	83	HIS	4.4
1	4-A	83	HIS	4.4
1	5-A	83	HIS	4.4
1	6-A	83	HIS	4.4
1	7-A	83	HIS	4.4
1	8-A	83	HIS	4.4
1	1-B	46	THR	4.4
1	2-B	46	THR	4.4
1	3-B	46	THR	4.4
1	4-B	46	THR	4.4
1	5-B	46	THR	4.4
1	6-B	46	THR	4.4
1	7-B	46	THR	4.4
1	8-B	46	THR	4.4
1	1-A	51	LYS	3.2
1	2-A	51	LYS	3.2
1	3-A	51	LYS	3.2
1	4-A	51	LYS	3.2
1	5-A	51	LYS	3.2
1	6-A	51	LYS	3.2
1	7-A	51	LYS	3.2

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Mol	Chain	Res	Type	RSRZ
1	8-A	51	LYS	3.2
1	1-B	48	PHE	3.2
1	2-B	48	PHE	3.2
1	3-B	48	PHE	3.2
1	4-B	48	PHE	3.2
1	5-B	48	PHE	3.2
1	6-B	48	PHE	3.2
1	7-B	48	PHE	3.2
1	8-B	48	PHE	3.2
1	1-A	44	ARG	3.1
1	2-A	44	ARG	3.1
1	3-A	44	ARG	3.1
1	4-A	44	ARG	3.1
1	5-A	44	ARG	3.1
1	6-A	44	ARG	3.1
1	7-A	44	ARG	3.1
1	8-A	44	ARG	3.1
1	1-B	50	SER	2.9
1	2-B	50	SER	2.9
1	3-B	50	SER	2.9
1	4-B	50	SER	2.9
1	5-B	50	SER	2.9
1	6-B	50	SER	2.9
1	7-B	50	SER	2.9
1	8-B	50	SER	2.9
1	1-A	48	PHE	2.8
1	2-A	48	PHE	2.8
1	3-A	48	PHE	2.8
1	4-A	48	PHE	2.8
1	5-A	48	PHE	2.8
1	6-A	48	PHE	2.8
1	7-A	48	PHE	2.8
1	8-A	48	PHE	2.8
1	1-B	86	ASN	2.6
1	2-B	86	ASN	2.6
1	3-B	86	ASN	2.6
1	4-B	86	ASN	2.6
1	5-B	86	ASN	2.6
1	6-B	86	ASN	2.6
1	7-B	86	ASN	2.6
1	8-B	86	ASN	2.6
1	1-B	62	SER	2.5

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Mol	Chain	Res	Type	RSRZ
1	2-B	62	SER	2.5
1	3-B	62	SER	2.5
1	4-B	62	SER	2.5
1	5-B	62	SER	2.5
1	6-B	62	SER	2.5
1	7-B	62	SER	2.5
1	8-B	62	SER	2.5
1	1-A	60	PRO	2.1
1	2-A	60	PRO	2.1
1	3-A	60	PRO	2.1
1	4-A	60	PRO	2.1
1	5-A	60	PRO	2.1
1	6-A	60	PRO	2.1
1	7-A	60	PRO	2.1
1	8-A	60	PRO	2.1

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
4	EDO	6-B	612	4/4	0.94	0.20	10.62	35,35,35,38	4
4	EDO	8-B	612	4/4	0.94	0.20	10.62	34,36,36,37	4
4	EDO	4-B	612	4/4	0.94	0.20	10.62	35,36,36,37	4
4	EDO	7-B	612	4/4	0.94	0.20	9.09	35,35,36,37	4
4	EDO	5-B	612	4/4	0.94	0.20	9.09	35,36,36,37	4
4	EDO	3-B	612	4/4	0.94	0.20	9.09	35,36,37,37	4

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
4	EDO	2-B	612	4/4	0.94	0.20	9.09	35,36,37,37	4
4	EDO	3-A	608	4/4	0.92	0.14	7.59	28,29,30,31	4
4	EDO	1-A	608	4/4	0.92	0.14	7.59	28,29,30,31	4
4	EDO	4-A	608	4/4	0.92	0.14	7.59	28,29,30,31	4
4	EDO	6-A	608	4/4	0.92	0.14	7.59	28,29,30,31	4
4	EDO	8-A	608	4/4	0.92	0.14	7.29	28,29,30,31	4
4	EDO	2-A	608	4/4	0.92	0.14	7.29	27,29,30,30	4
4	EDO	5-A	608	4/4	0.92	0.14	7.29	28,29,30,31	4
4	EDO	7-A	608	4/4	0.92	0.14	7.14	28,29,30,31	4
4	EDO	2-B	611	4/4	0.93	0.15	5.48	30,30,30,32	4
4	EDO	1-B	612	4/4	0.94	0.20	5.44	35,36,37,37	4
4	EDO	5-B	611	4/4	0.93	0.15	5.39	30,30,31,32	4
4	EDO	4-B	611	4/4	0.93	0.15	5.34	30,30,30,32	4
4	EDO	6-B	611	4/4	0.93	0.15	5.26	30,30,31,32	4
4	EDO	3-B	611	4/4	0.93	0.15	5.26	30,30,31,32	4
4	EDO	1-B	611	4/4	0.93	0.15	5.26	30,30,30,32	4
4	EDO	8-B	611	4/4	0.93	0.15	5.21	30,30,30,33	4
4	EDO	7-B	611	4/4	0.93	0.15	5.15	30,30,30,33	4
4	EDO	1-A	609	4/4	0.95	0.12	4.58	27,28,28,29	4
4	EDO	3-A	609	4/4	0.95	0.12	4.49	27,28,28,29	4
4	EDO	5-A	609	4/4	0.95	0.12	4.49	27,28,28,29	4
4	EDO	8-A	609	4/4	0.95	0.12	4.29	27,28,28,29	4
4	EDO	2-A	609	4/4	0.95	0.12	3.84	27,28,28,28	4
4	EDO	4-A	609	4/4	0.95	0.12	3.64	27,28,28,29	4
4	EDO	6-A	609	4/4	0.95	0.12	3.64	28,28,28,29	4
4	EDO	7-A	609	4/4	0.95	0.12	3.39	27,27,28,31	4
2	ZN	6-A	604	1/1	0.97	0.14	3.08	30,30,30,30	1
2	ZN	2-A	604	1/1	0.97	0.14	3.02	7,7,7,7	1
2	ZN	7-A	604	1/1	0.97	0.14	2.93	26,26,26,26	1
2	ZN	1-A	604	1/1	0.97	0.14	2.93	10,10,10,10	1
2	ZN	4-A	604	1/1	0.97	0.14	2.93	9,9,9,9	1
2	ZN	3-A	604	1/1	0.97	0.14	2.93	27,27,27,27	1
4	EDO	1-B	610	4/4	0.98	0.10	2.66	13,14,16,18	4
4	EDO	7-B	610	4/4	0.98	0.10	2.66	11,12,17,18	4
4	EDO	6-B	610	4/4	0.98	0.10	2.66	12,13,16,18	4
4	EDO	4-B	610	4/4	0.98	0.10	2.66	12,13,16,18	4
4	EDO	5-B	610	4/4	0.98	0.10	2.66	13,14,17,18	4
4	EDO	8-B	610	4/4	0.98	0.10	2.66	11,12,16,18	4
4	EDO	3-B	610	4/4	0.98	0.10	2.59	12,13,17,18	4
4	EDO	2-B	610	4/4	0.98	0.10	2.59	12,14,17,17	4
2	ZN	5-A	604	1/1	0.97	0.14	1.50	0,0,0,0	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	AMP	4-B	602	22/23	0.95	0.11	1.17	20,27,28,31	22
3	AMP	8-B	602	22/23	0.95	0.11	1.08	19,26,28,30	22
3	AMP	3-B	602	22/23	0.95	0.11	1.08	19,26,28,29	22
3	AMP	5-B	602	22/23	0.95	0.11	1.08	19,27,28,30	22
3	AMP	2-B	602	22/23	0.95	0.11	1.08	21,27,28,30	22
3	AMP	7-B	602	22/23	0.95	0.11	1.08	19,26,28,32	22
3	AMP	6-B	602	22/23	0.95	0.11	1.08	20,27,28,29	22
3	AMP	1-B	602	22/23	0.95	0.11	1.08	20,27,28,31	22
3	AMP	3-A	601	22/23	0.98	0.08	0.60	12,21,23,26	22
3	AMP	7-A	601	22/23	0.98	0.08	0.51	7,21,23,24	22
3	AMP	8-A	601	22/23	0.98	0.08	0.50	11,21,22,23	22
3	AMP	2-A	601	22/23	0.98	0.08	0.50	16,21,22,26	22
3	AMP	6-A	601	22/23	0.98	0.08	0.50	13,21,22,24	22
3	AMP	1-A	601	22/23	0.98	0.08	0.50	16,21,22,27	22
3	AMP	5-A	601	22/23	0.98	0.08	0.50	3,21,22,23	22
3	AMP	4-A	601	22/23	0.98	0.08	0.45	12,21,24,24	22
4	EDO	1-A	607	4/4	0.99	0.06	-0.04	10,11,12,13	4
4	EDO	3-A	607	4/4	0.99	0.06	-0.04	12,12,12,13	4
4	EDO	2-A	607	4/4	0.99	0.06	-0.06	10,11,13,13	4
4	EDO	8-A	607	4/4	0.99	0.06	-0.06	11,12,12,12	4
4	EDO	4-A	607	4/4	0.99	0.06	-0.06	10,11,12,13	4
4	EDO	5-A	607	4/4	0.99	0.06	-0.06	11,12,12,13	4
4	EDO	7-A	607	4/4	0.99	0.06	-0.06	9,11,12,13	4
4	EDO	6-A	607	4/4	0.99	0.06	-0.06	11,12,12,13	4
2	ZN	5-B	606	1/1	1.00	0.05	-0.68	24,24,24,24	1
2	ZN	2-B	606	1/1	1.00	0.05	-0.86	18,18,18,18	1
2	ZN	3-B	606	1/1	1.00	0.05	-0.86	24,24,24,24	1
2	ZN	1-B	606	1/1	1.00	0.05	-0.86	24,24,24,24	1
2	ZN	6-B	606	1/1	1.00	0.05	-0.89	13,13,13,13	1
2	ZN	4-B	606	1/1	1.00	0.05	-0.91	23,23,23,23	1
2	ZN	8-B	606	1/1	1.00	0.05	-0.97	25,25,25,25	1
2	ZN	1-B	605	1/1	1.00	0.03	-1.75	10,10,10,10	1
2	ZN	5-B	605	1/1	1.00	0.03	-1.75	19,19,19,19	1
2	ZN	8-B	605	1/1	1.00	0.03	-1.75	7,7,7,7	1
2	ZN	2-B	605	1/1	1.00	0.03	-1.75	19,19,19,19	1
2	ZN	4-B	605	1/1	1.00	0.03	-1.77	13,13,13,13	1
2	ZN	6-B	605	1/1	1.00	0.03	-1.77	13,13,13,13	1
2	ZN	7-B	605	1/1	1.00	0.03	-1.77	11,11,11,11	1
2	ZN	3-B	605	1/1	1.00	0.03	-1.77	14,14,14,14	1
2	ZN	1-A	603	1/1	1.00	0.04	-2.04	11,11,11,11	1
2	ZN	2-A	603	1/1	1.00	0.04	-2.41	24,24,24,24	1
2	ZN	3-A	603	1/1	1.00	0.04	-2.41	25,25,25,25	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	ZN	8-A	603	1/1	1.00	0.04	-2.41	24,24,24,24	1
2	ZN	4-A	603	1/1	1.00	0.04	-2.41	10,10,10,10	1
2	ZN	6-A	603	1/1	1.00	0.04	-2.41	24,24,24,24	1
2	ZN	5-A	603	1/1	1.00	0.04	-2.64	23,23,23,23	1
2	ZN	7-A	603	1/1	1.00	0.04	-2.64	8,8,8,8	1
2	ZN	7-B	606	1/1	1.00	0.05	-	12,12,12,12	1
2	ZN	8-A	604	1/1	0.97	0.14	-	2,2,2,2	1

## 6.5 Other polymers [i](#)

There are no such residues in this entry.