



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 03:17 AM GMT

PDB ID : 3L2G  
Title : Glycocyamine kinase, beta-beta homodimer from marine worm *Namalycastis* sp., with transition state analog Mg(II)-ADP-NO<sub>3</sub>-glycocyamine.Part 2.  
Authors : Lim, K.; Pullalarevu, S.; Herzberg, O.  
Deposited on : 2009-12-15  
Resolution : 2.30 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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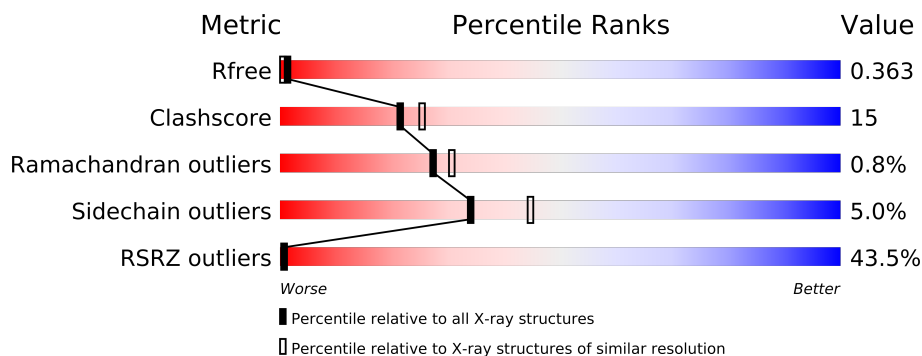
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.30 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))
$R_{free}$	66092	2929 (2.30-2.30)
Clashscore	79885	3679 (2.30-2.30)
Ramachandran outliers	78287	3642 (2.30-2.30)
Sidechain outliers	78261	3641 (2.30-2.30)
RSRZ outliers	66119	2930 (2.30-2.30)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	390	
1	B	390	
1	C	390	
1	D	390	
1	E	390	
1	F	390	
1	G	390	
1	H	390	
1	I	390	
1	J	390	
1	K	390	
1	L	390	
1	M	390	
1	N	390	

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Mol	Chain	Length	Quality of chain
1	O	390	
1	P	390	
1	Q	390	
1	R	390	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	NMG	B	502	-	X
2	NMG	D	504	-	X
2	NMG	N	514	-	X
2	NMG	Q	517	-	X
4	MG	G	707	-	X
4	MG	R	718	-	X
5	NO3	A	801	X	X
5	NO3	B	802	X	-
5	NO3	C	803	X	-
5	NO3	D	804	X	-
5	NO3	E	805	X	-
5	NO3	F	806	X	-
5	NO3	G	807	X	X
5	NO3	H	808	X	-
5	NO3	I	809	X	X
5	NO3	J	810	X	X
5	NO3	K	811	X	-
5	NO3	L	812	X	-
5	NO3	M	813	X	-
5	NO3	N	814	X	-
5	NO3	O	815	X	-
5	NO3	P	816	X	-
5	NO3	Q	817	X	-
5	NO3	R	818	X	-

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 56636 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Glycocyamine kinase beta chain.

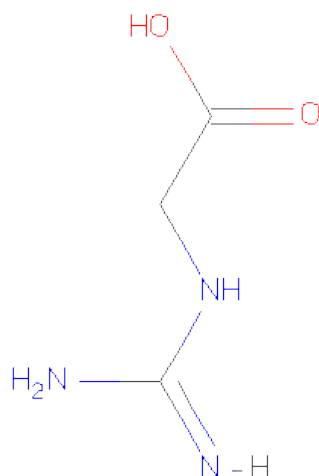
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	367	Total	C	N	O	S	0	0	0
			2910	1834	513	542	21			
1	B	388	Total	C	N	O	S	0	0	0
			3080	1942	544	573	21			
1	C	367	Total	C	N	O	S	0	0	0
			2910	1834	513	542	21			
1	D	385	Total	C	N	O	S	0	0	0
			3061	1930	541	569	21			
1	E	367	Total	C	N	O	S	0	0	0
			2910	1834	513	542	21			
1	F	382	Total	C	N	O	S	0	0	0
			3032	1912	537	562	21			
1	G	367	Total	C	N	O	S	0	0	0
			2910	1834	513	542	21			
1	H	382	Total	C	N	O	S	0	0	0
			3032	1912	537	562	21			
1	I	367	Total	C	N	O	S	0	0	0
			2910	1834	513	542	21			
1	J	385	Total	C	N	O	S	0	0	0
			3061	1930	541	569	21			
1	K	367	Total	C	N	O	S	0	0	0
			2910	1834	513	542	21			
1	L	381	Total	C	N	O	S	0	0	0
			3021	1903	536	561	21			
1	M	367	Total	C	N	O	S	0	0	0
			2910	1834	513	542	21			
1	N	382	Total	C	N	O	S	0	0	0
			3032	1912	537	562	21			
1	O	367	Total	C	N	O	S	0	0	0
			2910	1834	513	542	21			
1	P	382	Total	C	N	O	S	0	0	0
			3032	1912	537	562	21			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	366	Total	C	N	O	S	0	0	0
			2901	1828	511	541	21			
1	R	381	Total	C	N	O	S	0	0	0
			3021	1903	536	561	21			

- Molecule 2 is GUANIDINO ACETATE (three-letter code: NMG) (formula:  $C_3H_7N_3O_2$ ).



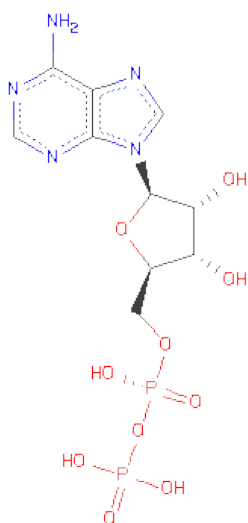
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			8	3	3	2		
2	B	1	Total	C	N	O	0	0
			8	3	3	2		
2	C	1	Total	C	N	O	0	0
			8	3	3	2		
2	D	1	Total	C	N	O	0	0
			8	3	3	2		
2	E	1	Total	C	N	O	0	0
			8	3	3	2		
2	F	1	Total	C	N	O	0	0
			8	3	3	2		
2	G	1	Total	C	N	O	0	0
			8	3	3	2		
2	H	1	Total	C	N	O	0	0
			8	3	3	2		
2	I	1	Total	C	N	O	0	0
			8	3	3	2		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	J	1	Total	C	N	O	0	0
			8	3	3	2		
2	K	1	Total	C	N	O	0	0
			8	3	3	2		
2	L	1	Total	C	N	O	0	0
			8	3	3	2		
2	M	1	Total	C	N	O	0	0
			8	3	3	2		
2	N	1	Total	C	N	O	0	0
			8	3	3	2		
2	O	1	Total	C	N	O	0	0
			8	3	3	2		
2	P	1	Total	C	N	O	0	0
			8	3	3	2		
2	Q	1	Total	C	N	O	0	0
			8	3	3	2		
2	R	1	Total	C	N	O	0	0
			8	3	3	2		

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	E	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	F	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	G	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	H	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	I	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	J	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	K	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	L	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	M	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	N	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	O	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	P	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	Q	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	R	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	P	1	Total	Mg	0	0
			1	1		
4	G	1	Total	Mg	0	0
			1	1		
4	J	1	Total	Mg	0	0
			1	1		

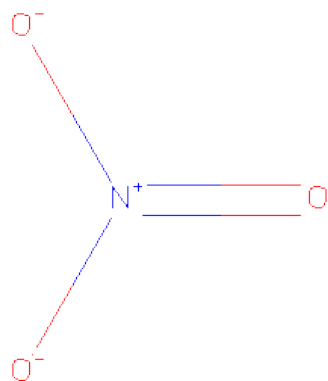
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	Q	1	Total 1	Mg 1	0	0
4	D	1	Total 1	Mg 1	0	0
4	K	1	Total 1	Mg 1	0	0
4	E	1	Total 1	Mg 1	0	0
4	H	1	Total 1	Mg 1	0	0
4	B	1	Total 1	Mg 1	0	0
4	I	1	Total 1	Mg 1	0	0
4	C	1	Total 1	Mg 1	0	0
4	A	1	Total 1	Mg 1	0	0
4	N	1	Total 1	Mg 1	0	0
4	O	1	Total 1	Mg 1	0	0
4	R	1	Total 1	Mg 1	0	0
4	L	1	Total 1	Mg 1	0	0
4	F	1	Total 1	Mg 1	0	0
4	M	1	Total 1	Mg 1	0	0

- Molecule 5 is NITRATE ION (three-letter code: NO3) (formula: NO<sub>3</sub>).





Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	N	O	0	0
			4	1	3		
5	B	1	Total	N	O	0	0
			4	1	3		
5	C	1	Total	N	O	0	0
			4	1	3		
5	D	1	Total	N	O	0	0
			4	1	3		
5	E	1	Total	N	O	0	0
			4	1	3		
5	F	1	Total	N	O	0	0
			4	1	3		
5	G	1	Total	N	O	0	0
			4	1	3		
5	H	1	Total	N	O	0	0
			4	1	3		
5	I	1	Total	N	O	0	0
			4	1	3		
5	J	1	Total	N	O	0	0
			4	1	3		
5	K	1	Total	N	O	0	0
			4	1	3		
5	L	1	Total	N	O	0	0
			4	1	3		
5	M	1	Total	N	O	0	0
			4	1	3		
5	N	1	Total	N	O	0	0
			4	1	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	O	1	Total	N	O	0	0
			4	1	3		
5	P	1	Total	N	O	0	0
			4	1	3		
5	Q	1	Total	N	O	0	0
			4	1	3		
5	R	1	Total	N	O	0	0
			4	1	3		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	99	Total	O	0	0
			99	99		
6	B	130	Total	O	0	0
			130	130		
6	C	155	Total	O	0	0
			155	155		
6	D	110	Total	O	0	0
			110	110		
6	E	117	Total	O	0	0
			117	117		
6	F	144	Total	O	0	0
			144	144		
6	G	133	Total	O	0	0
			133	133		
6	H	145	Total	O	0	0
			145	145		
6	I	118	Total	O	0	0
			118	118		
6	J	145	Total	O	0	0
			145	145		
6	K	127	Total	O	0	0
			127	127		
6	L	90	Total	O	0	0
			90	90		
6	M	143	Total	O	0	0
			143	143		
6	N	114	Total	O	0	0
			114	114		
6	O	173	Total	O	0	0
			173	173		

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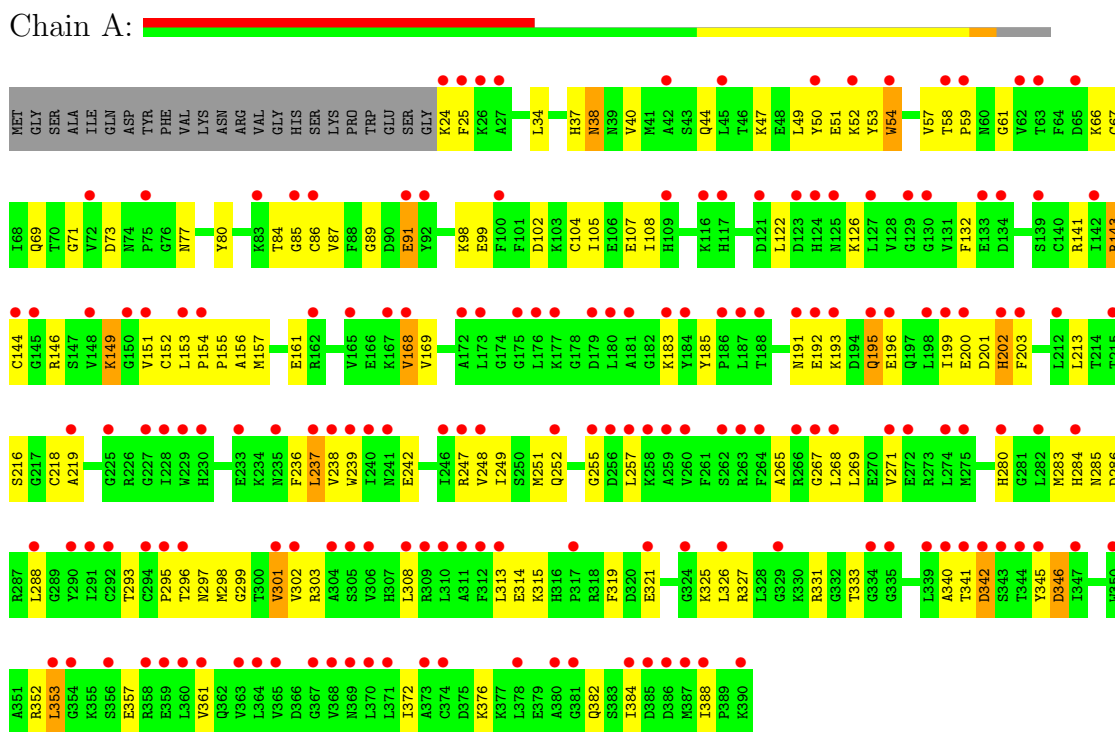
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	P	149	Total 149	O 149	0	0
6	Q	105	Total 105	O 105	0	0
6	R	166	Total 166	O 166	0	0

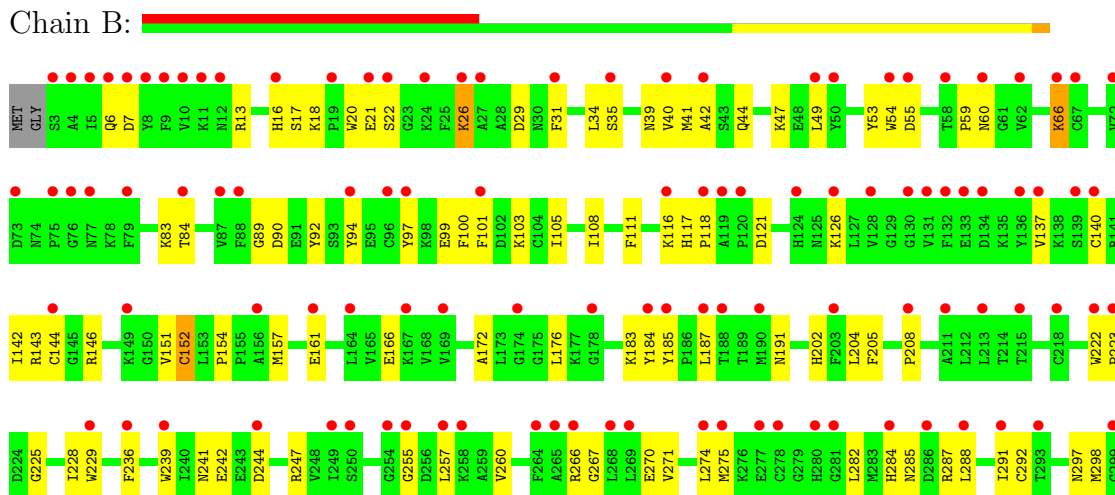
### 3 Residue-property plots

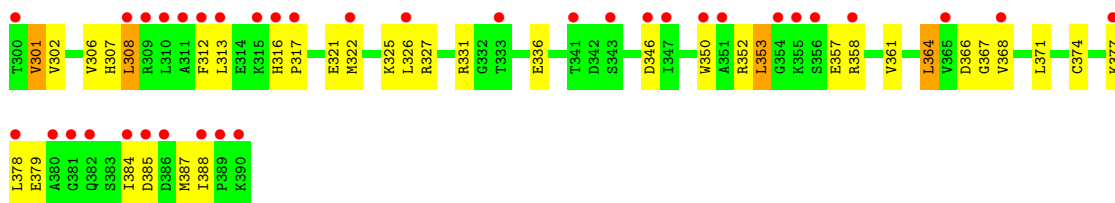
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

- Molecule 1: Glycocyamine kinase beta chain



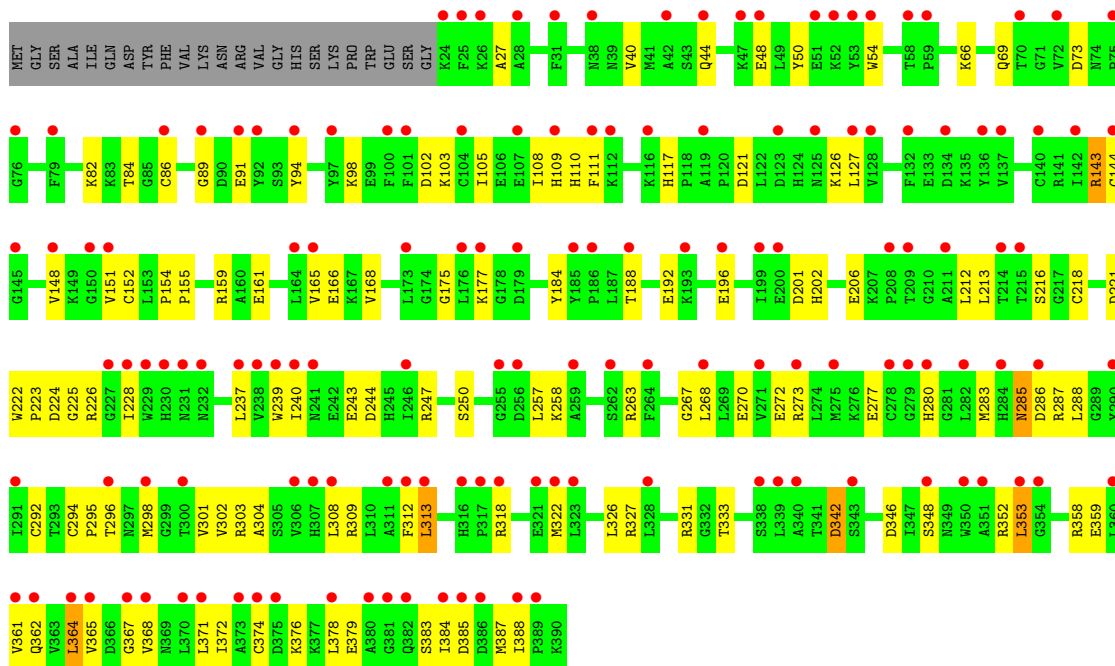
- Molecule 1: Glycocyamine kinase beta chain





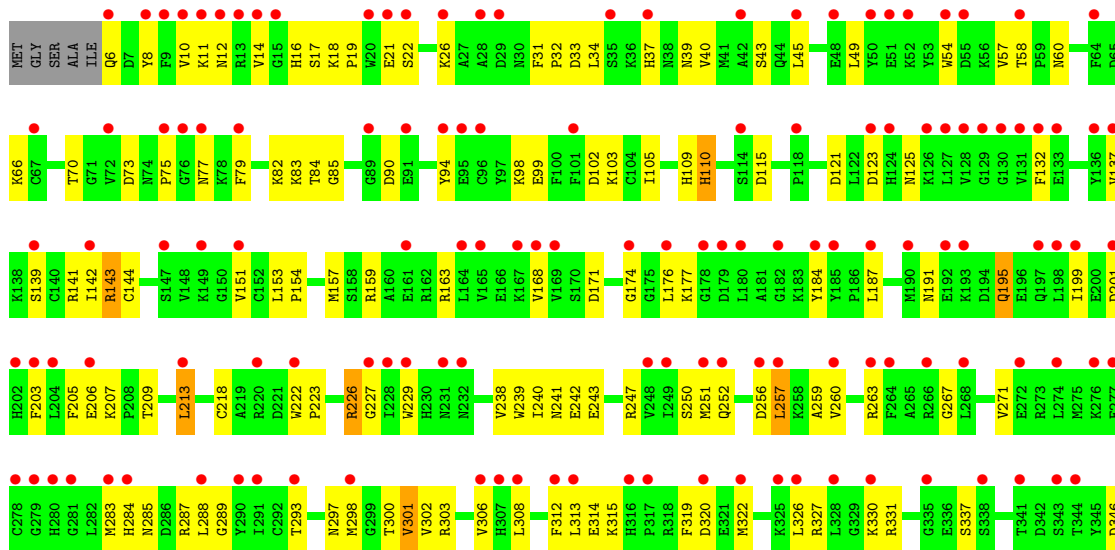
• Molecule 1: Glycocyamine kinase beta chain

Chain C:



• Molecule 1: Glycocyamine kinase beta chain

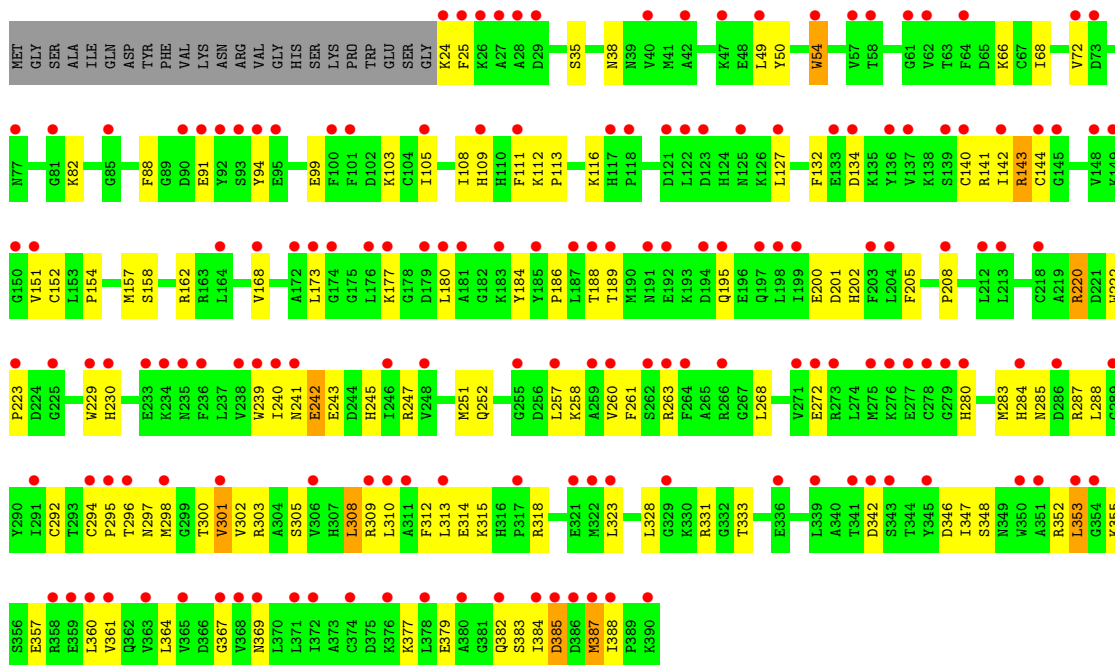
Chain D:





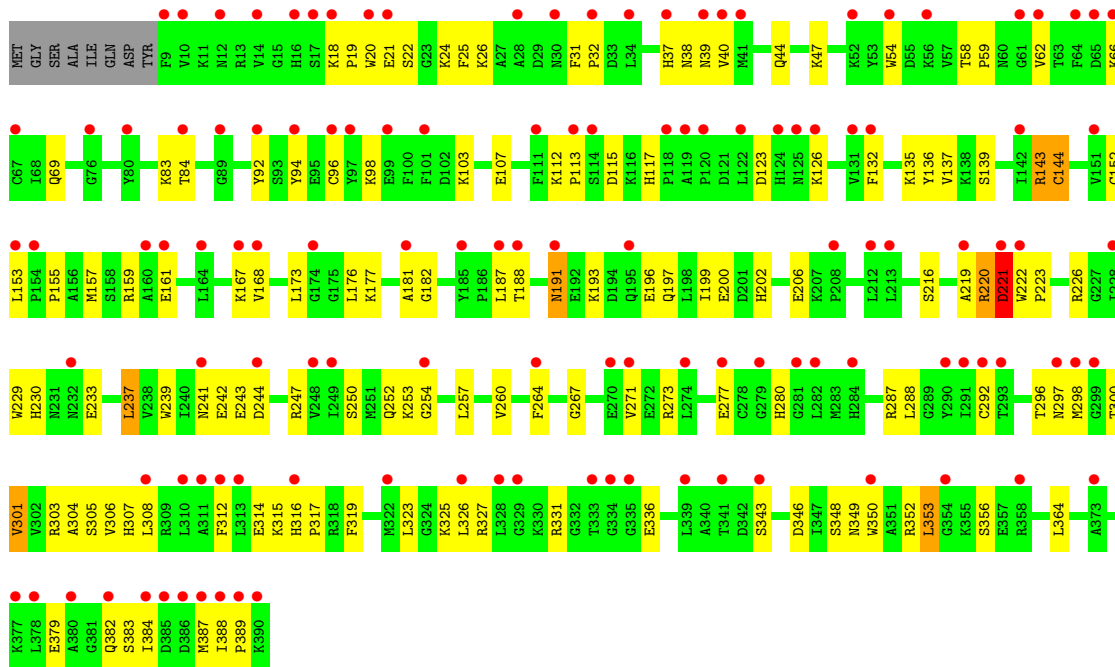
• Molecule 1: Glycocyamine kinase beta chain

Chain E:



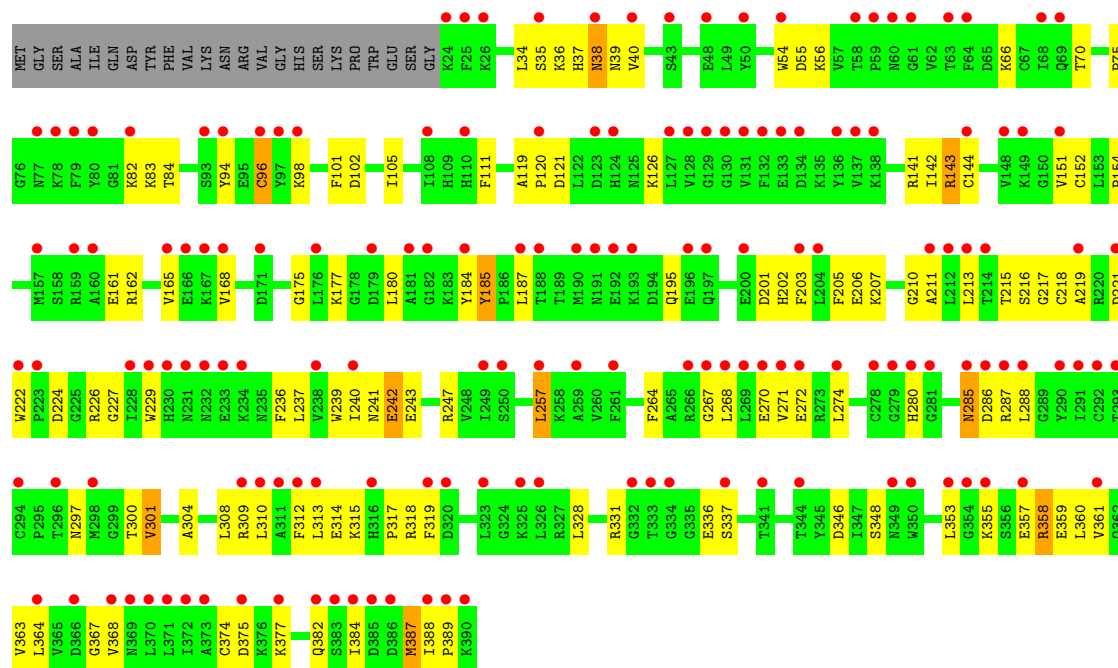
• Molecule 1: Glycocyamine kinase beta chain

Chain F:



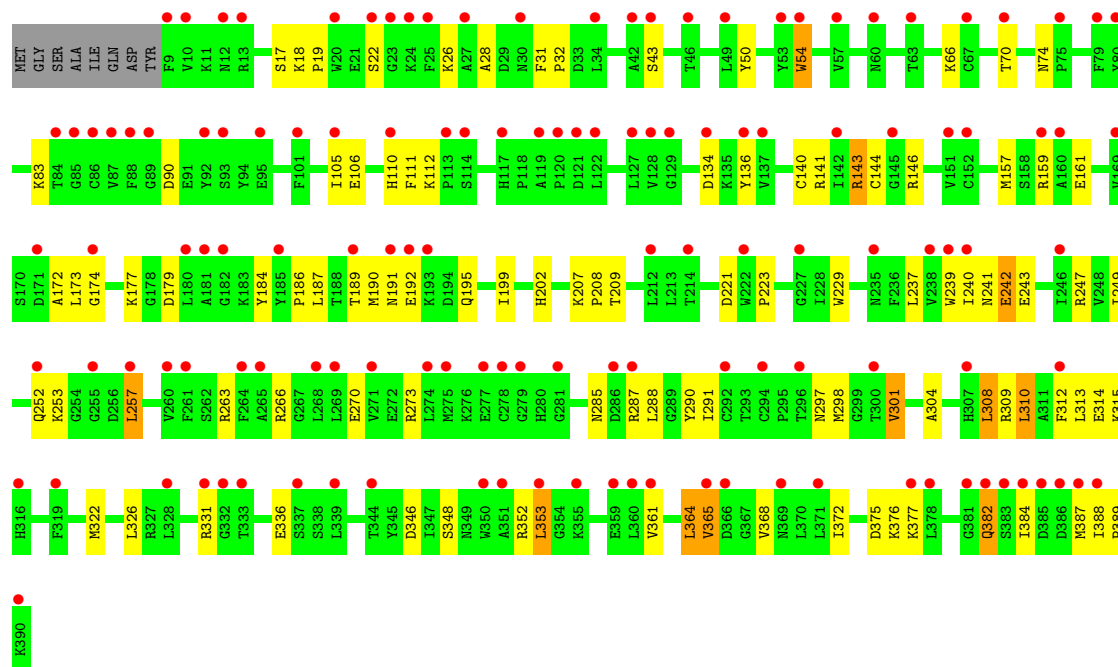
• Molecule 1: Glycocyamine kinase beta chain

Chain G:



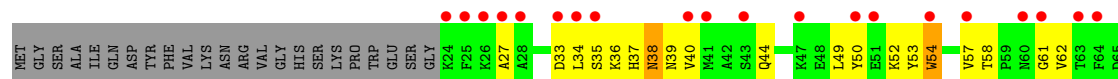
- Molecule 1: Glycocyamine kinase beta chain

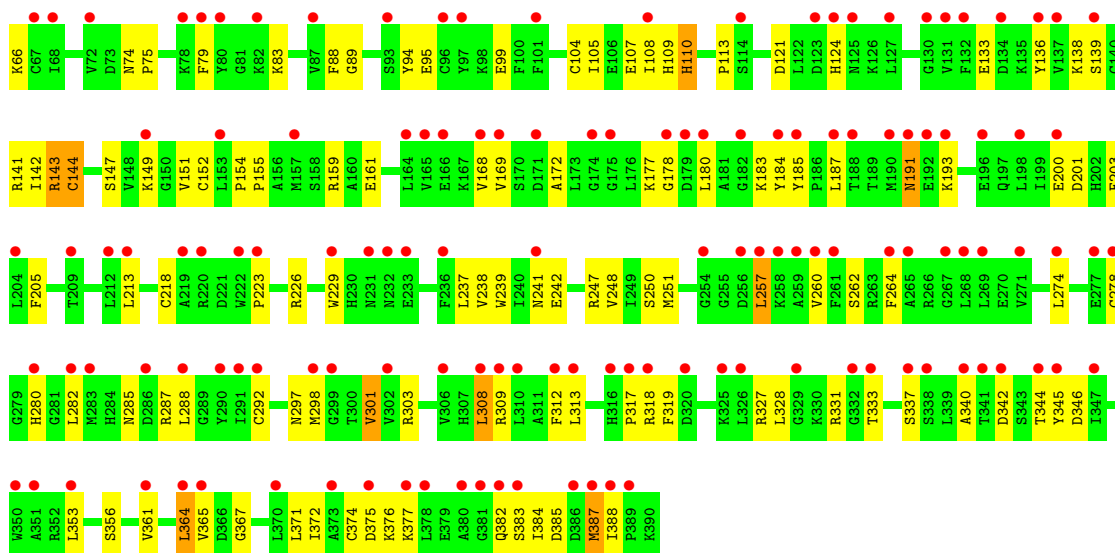
Chain H:



- Molecule 1: Glycocyamine kinase beta chain

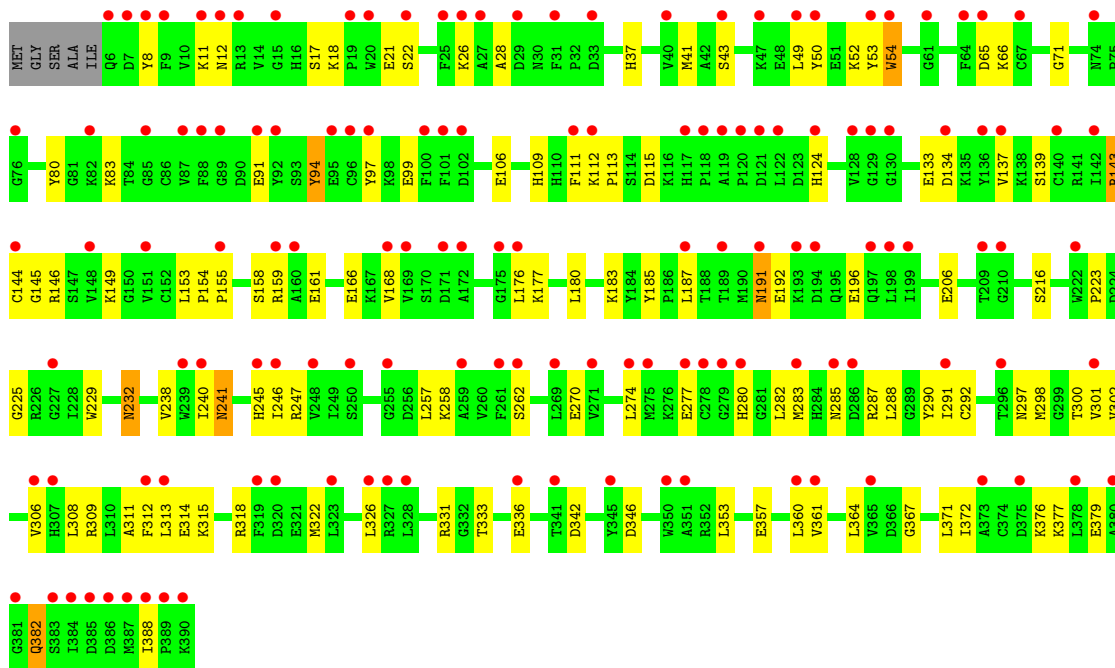
Chain I:





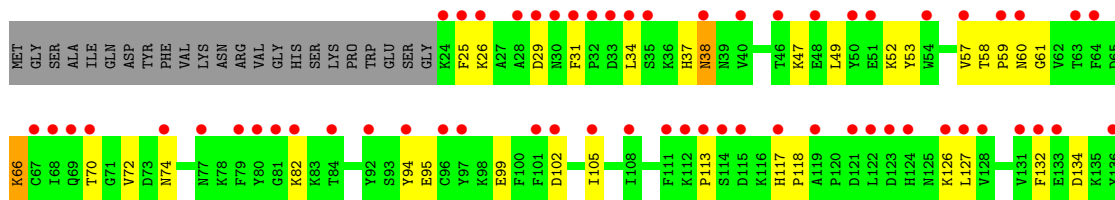
• Molecule 1: Glycocyamine kinase beta chain

Chain J: 

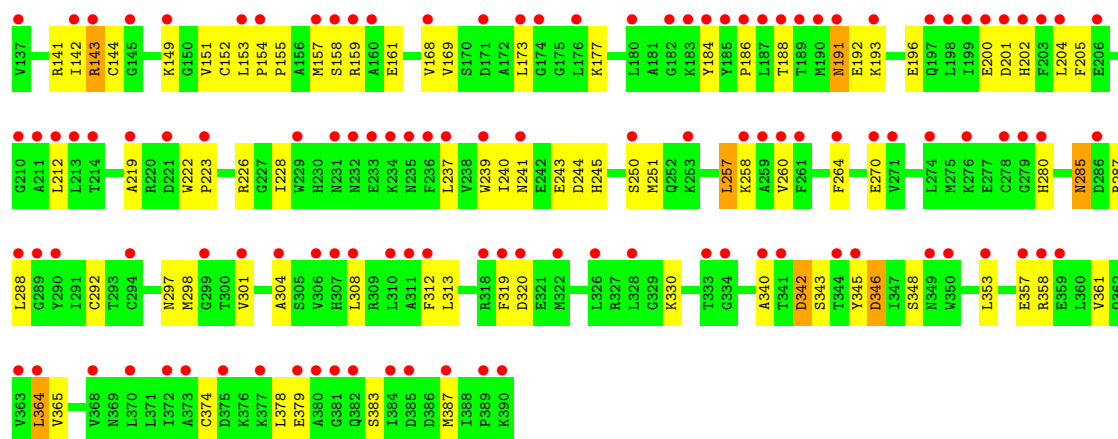


• Molecule 1: Glycocyamine kinase beta chain

Chain K: 

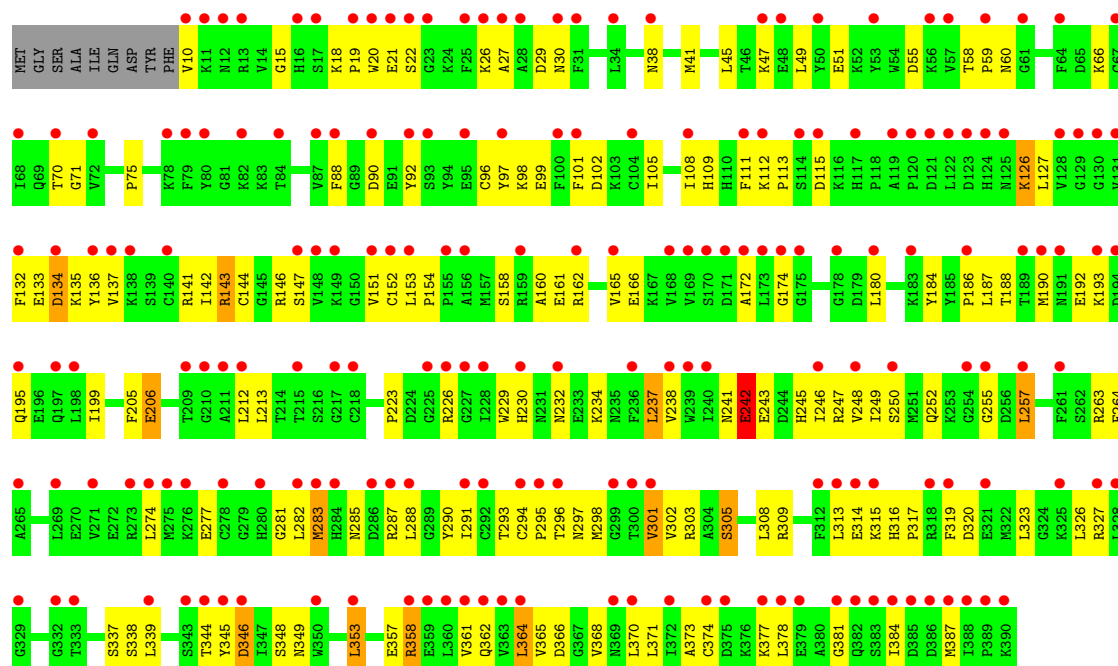






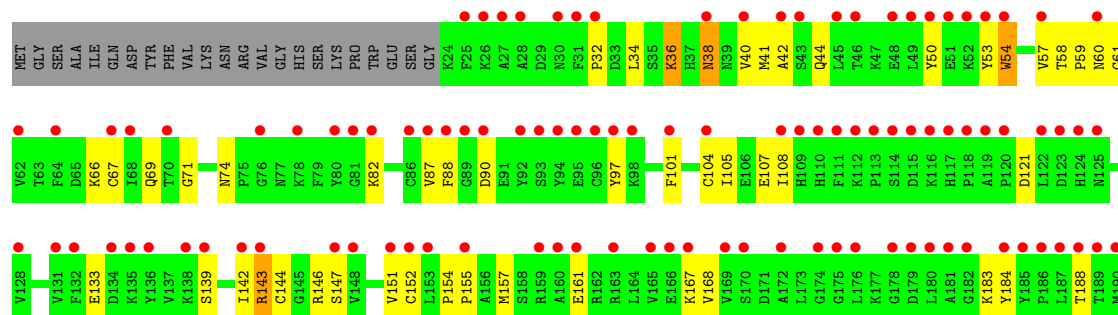
• Molecule 1: Glycocyamine kinase beta chain

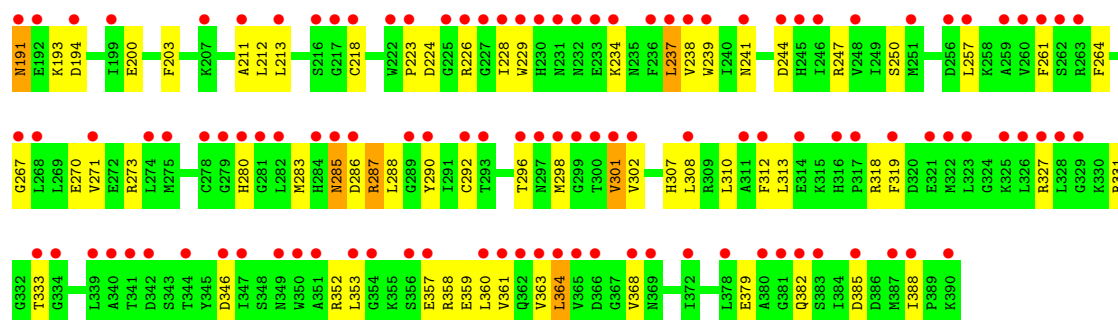
Chain L:



• Molecule 1: Glycocyamine kinase beta chain

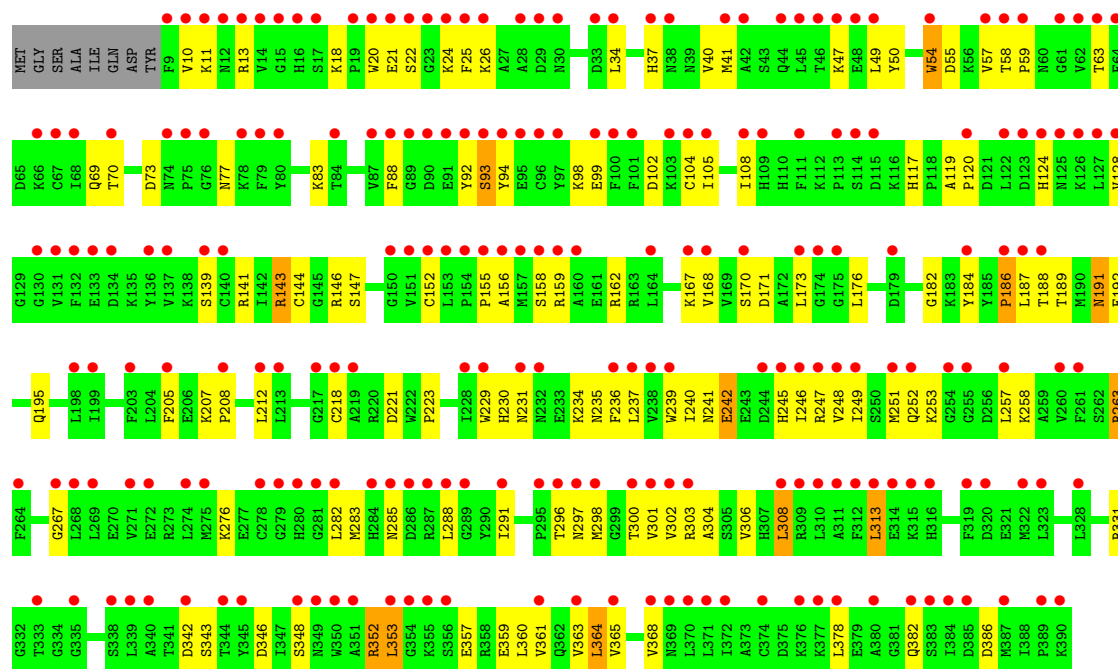
Chain M:





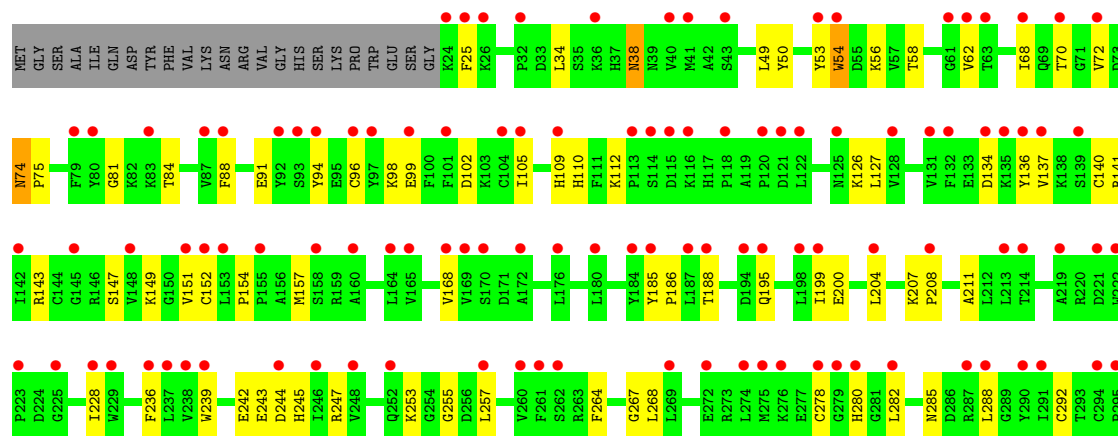
• Molecule 1: Glycocyamine kinase beta chain

Chain N:

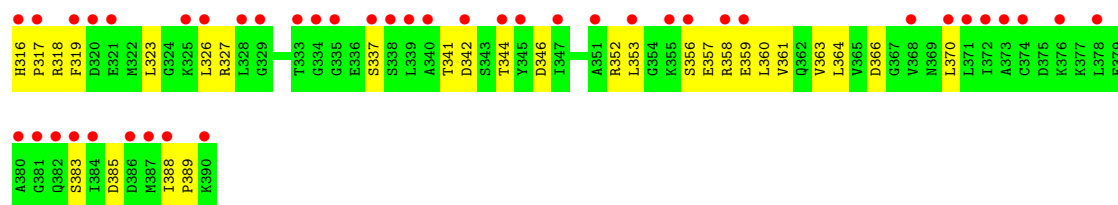


• Molecule 1: Glycocyamine kinase beta chain

Chain O:

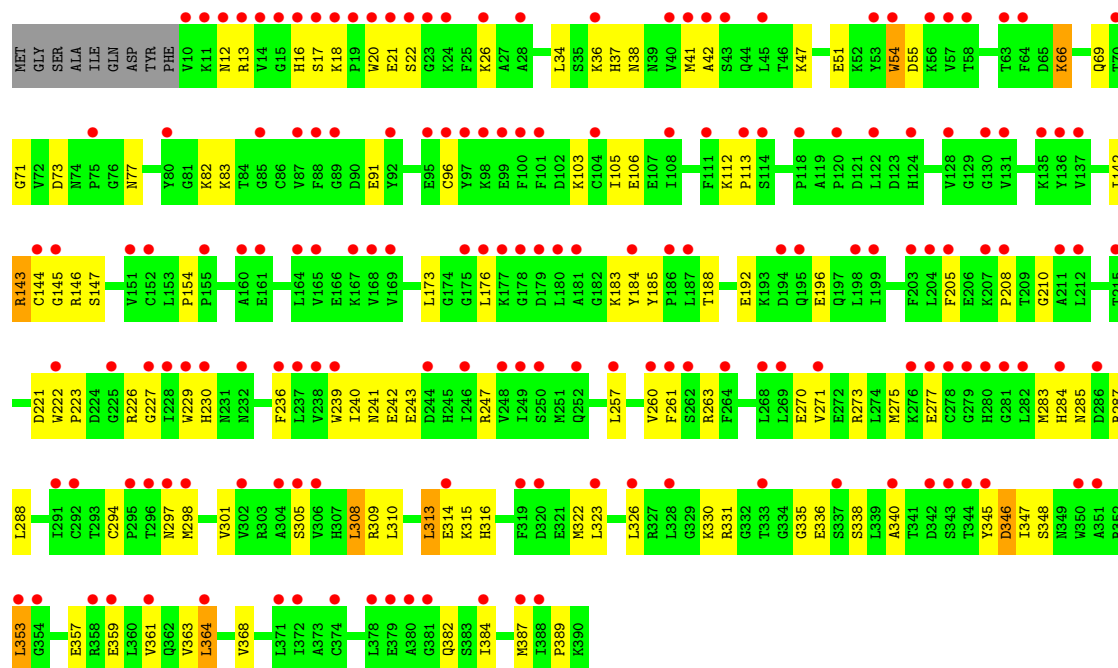






● Molecule 1: Glycocyamine kinase beta chain

Chain R:



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	243.11Å 114.27Å 259.90Å 90.00° 90.25° 90.00°	Depositor
Resolution (Å)	20.00 – 2.30 33.05 – 2.30	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-2.30) 92.1 (33.05-2.30)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.08 (at 2.29Å)	Xtriage
Refinement program	phenix	Depositor
R, $R_{free}$	0.197 , 0.263 0.347 , 0.363	Depositor DCC
$R_{free}$ test set	29382 reflections (5.27%)	DCC
Wilson B-factor (Å <sup>2</sup> )	23.1	Xtriage
Anisotropy	0.184	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 17.1	EDS
Estimated twinning fraction	0.428 for h,-k,-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	38 of 610844 reflections (0.006%)	Xtriage
$F_o, F_c$ correlation	0.75	EDS
Total number of atoms	56636	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 38.54 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 3.6323e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NMG, MG, ADP, NO3

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	A	0.33	0/2972	0.51	0/3997
1	B	0.36	0/3148	0.55	1/4235 (0.0%)
1	C	0.34	0/2972	0.53	0/3997
1	D	0.36	0/3129	0.54	0/4209
1	E	0.34	0/2972	0.52	0/3997
1	F	0.38	0/3099	0.56	0/4168
1	G	0.35	0/2972	0.52	0/3997
1	H	0.38	0/3099	0.55	0/4168
1	I	0.36	0/2972	0.54	0/3997
1	J	0.37	0/3129	0.55	0/4209
1	K	0.35	0/2972	0.54	0/3997
1	L	0.36	0/3087	0.54	0/4152
1	M	0.34	0/2972	0.53	0/3997
1	N	0.35	0/3099	0.54	0/4168
1	O	0.36	0/2972	0.54	0/3997
1	P	0.37	0/3099	0.55	0/4168
1	Q	0.34	0/2963	0.53	0/3986
1	R	0.39	0/3087	0.57	1/4152 (0.0%)
All	All	0.36	0/54715	0.54	2/73591 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	308	LEU	CA-CB-CG	5.41	127.75	115.30
1	R	353	LEU	CA-CB-CG	5.04	126.90	115.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2910	0	2879	90	0
1	B	3080	0	3039	97	0
1	C	2910	0	2879	90	0
1	D	3061	0	3018	115	0
1	E	2910	0	2879	97	0
1	F	3032	0	2997	109	0
1	G	2910	0	2879	90	0
1	H	3032	0	2997	81	0
1	I	2910	0	2879	107	0
1	J	3061	0	3018	78	0
1	K	2910	0	2879	92	0
1	L	3021	0	2988	119	0
1	M	2910	0	2879	83	0
1	N	3032	0	2997	101	0
1	O	2910	0	2879	71	0
1	P	3032	0	2997	77	0
1	Q	2901	0	2866	95	0
1	R	3021	0	2988	85	0
2	A	8	0	5	0	0
2	B	8	0	5	1	0
2	C	8	0	5	0	0
2	D	8	0	5	1	0
2	E	8	0	5	0	0
2	F	8	0	5	0	0
2	G	8	0	5	0	0
2	H	8	0	5	1	0
2	I	8	0	5	0	0
2	J	8	0	5	1	0
2	K	8	0	5	0	0
2	L	8	0	5	0	0
2	M	8	0	5	0	0
2	N	8	0	5	0	0
2	O	8	0	5	2	0
2	P	8	0	5	0	0
2	Q	8	0	5	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	R	8	0	5	1	0
3	A	27	0	12	3	0
3	B	27	0	12	4	0
3	C	27	0	12	1	0
3	D	27	0	12	3	0
3	E	27	0	12	4	0
3	F	27	0	12	4	0
3	G	27	0	12	3	0
3	H	27	0	12	2	0
3	I	27	0	12	2	0
3	J	27	0	12	2	0
3	K	27	0	12	1	0
3	L	27	0	12	2	0
3	M	27	0	12	4	0
3	N	27	0	12	3	0
3	O	27	0	12	2	0
3	P	27	0	12	2	0
3	Q	27	0	12	3	0
3	R	27	0	12	3	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
4	G	1	0	0	0	0
4	H	1	0	0	0	0
4	I	1	0	0	0	0
4	J	1	0	0	0	0
4	K	1	0	0	0	0
4	L	1	0	0	0	0
4	M	1	0	0	0	0
4	N	1	0	0	0	0
4	O	1	0	0	0	0
4	P	1	0	0	0	0
4	Q	1	0	0	0	0
4	R	1	0	0	0	0
5	A	4	0	0	0	0
5	B	4	0	0	1	0
5	C	4	0	0	0	0
5	D	4	0	0	1	0
5	E	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	F	4	0	0	0	0
5	G	4	0	0	0	0
5	H	4	0	0	1	0
5	I	4	0	0	0	0
5	J	4	0	0	0	0
5	K	4	0	0	1	0
5	L	4	0	0	0	0
5	M	4	0	0	0	0
5	N	4	0	0	0	0
5	O	4	0	0	0	0
5	P	4	0	0	0	0
5	Q	4	0	0	0	0
5	R	4	0	0	1	0
6	A	99	0	0	2	0
6	B	130	0	0	2	0
6	C	155	0	0	4	0
6	D	110	0	0	12	0
6	E	117	0	0	7	0
6	F	144	0	0	6	0
6	G	133	0	0	5	0
6	H	145	0	0	13	0
6	I	118	0	0	9	0
6	J	145	0	0	7	0
6	K	127	0	0	4	0
6	L	90	0	0	6	0
6	M	143	0	0	9	0
6	N	114	0	0	6	0
6	O	173	0	0	6	0
6	P	149	0	0	9	0
6	Q	105	0	0	13	0
6	R	166	0	0	10	0
All	All	56636	0	53243	1649	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 15.

All (1649) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:126:LYS:HB2	1:C:358:ARG:HD2	1.39	1.02
1:B:285:ASN:HD22	1:B:288:LEU:H	1.06	1.00
1:K:191:ASN:HD21	1:K:193:LYS:HB2	1.29	0.97
1:D:285:ASN:HD22	1:D:288:LEU:H	1.02	0.94

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:J:285:ASN:HD22	1:J:288:LEU:H	1.11	0.92
1:F:305:SER:HB3	1:F:348:SER:HB3	1.52	0.91
1:N:285:ASN:HD22	1:N:288:LEU:H	1.14	0.90
1:H:285:ASN:HD22	1:H:288:LEU:H	1.22	0.87
1:L:134:ASP:HB2	6:L:1785:HOH:O	1.74	0.86
1:A:191:ASN:HD21	1:A:193:LYS:HB2	1.41	0.86
1:I:285:ASN:HD22	1:I:288:LEU:H	1.24	0.86
1:Q:285:ASN:HD22	1:Q:288:LEU:H	1.25	0.85
1:L:188:THR:HG22	1:L:223:PRO:HG2	1.57	0.84
1:D:285:ASN:HD22	1:D:288:LEU:N	1.75	0.84
1:F:253:LYS:HE2	6:F:1801:HOH:O	1.78	0.84
1:N:285:ASN:ND2	1:N:288:LEU:HG	1.93	0.83
1:G:285:ASN:ND2	1:G:287:ARG:H	1.76	0.82
1:M:239:TRP:HB2	1:M:247:ARG:HB2	1.59	0.82
1:L:298:MET:HE3	1:L:353:LEU:HD12	1.62	0.81
1:O:239:TRP:HB2	1:O:247:ARG:HB2	1.63	0.81
1:F:159:ARG:HG3	1:F:221:ASP:OD2	1.79	0.81
1:H:285:ASN:HD22	1:H:288:LEU:N	1.78	0.81
1:P:377:LYS:HG3	1:P:387:MET:HE1	1.60	0.81
1:B:208:PRO:HG3	1:B:222:TRP:CE2	2.15	0.80
1:L:314:GLU:HB2	1:L:345:TYR:OH	1.80	0.80
1:G:101:PHE:O	1:G:105:ILE:HG13	1.81	0.80
1:G:213:LEU:HD12	1:G:218:CYS:HB2	1.62	0.80
1:E:168:VAL:HG13	1:E:280:HIS:CE1	2.18	0.79
1:L:285:ASN:HD22	1:L:288:LEU:H	1.31	0.78
1:M:285:ASN:HD22	1:M:286:ASP:N	1.80	0.78
1:N:364:LEU:O	1:N:368:VAL:HG23	1.82	0.78
1:Q:359:GLU:O	1:Q:363:VAL:HG23	1.83	0.78
1:L:297:ASN:HB3	1:L:301:VAL:HG13	1.64	0.78
1:A:298:MET:HE3	1:A:353:LEU:HD12	1.64	0.77
1:Q:196:GLU:O	1:Q:200:GLU:HB2	1.84	0.77
1:G:331:ARG:HB2	1:G:346:ASP:HB3	1.67	0.77
1:M:285:ASN:ND2	1:M:287:ARG:H	1.81	0.77
1:J:113:PRO:HA	1:J:287:ARG:NH2	1.99	0.77
1:P:123:ASP:OD1	1:P:125:ASN:HB2	1.84	0.77
1:G:285:ASN:HD22	1:G:287:ARG:H	1.31	0.77
1:C:44:GLN:OE1	1:C:103:LYS:HE3	1.85	0.76
1:L:285:ASN:HB2	1:L:291:ILE:HD11	1.66	0.76
1:K:49:LEU:HD21	1:K:99:GLU:HG2	1.65	0.76
1:M:191:ASN:ND2	1:M:193:LYS:H	1.83	0.76
1:I:40:VAL:HG13	1:I:107:GLU:OE1	1.86	0.76
1:A:341:THR:O	1:A:342:ASP:HB2	1.86	0.76

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:L:58:THR:HG22	1:L:96:CYS:SG	2.26	0.75
1:B:285:ASN:ND2	1:B:288:LEU:H	1.83	0.75
1:L:247:ARG:HD2	6:L:2685:HOH:O	1.85	0.75
1:R:188:THR:HG22	1:R:223:PRO:HG2	1.68	0.75
1:M:188:THR:HG23	6:M:1774:HOH:O	1.86	0.75
1:A:321:GLU:O	1:A:325:LYS:HG3	1.87	0.75
1:N:302:VAL:O	1:N:352:ARG:HD3	1.86	0.75
1:P:188:THR:HG23	6:P:1507:HOH:O	1.86	0.74
1:A:191:ASN:ND2	1:A:193:LYS:HB2	2.02	0.74
1:O:305:SER:HB3	1:O:348:SER:HB3	1.68	0.74
1:I:187:LEU:HD23	1:I:223:PRO:HB3	1.69	0.74
1:O:152:CYS:SG	1:P:17:SER:HB3	2.28	0.74
1:F:188:THR:HG23	6:F:1709:HOH:O	1.87	0.73
1:R:357:GLU:O	1:R:361:VAL:HG23	1.88	0.73
1:F:18:LYS:HD3	1:F:20:TRP:CZ2	2.23	0.73
1:K:38:ASN:HD21	1:K:82:LYS:HG3	1.54	0.73
1:C:239:TRP:HB2	1:C:247:ARG:HB2	1.71	0.73
1:O:314:GLU:HG2	1:O:315:LYS:HD2	1.70	0.73
1:I:317:PRO:HB2	1:Q:253:LYS:HD2	1.71	0.73
1:L:384:ILE:HA	1:L:387:MET:HG3	1.69	0.73
1:B:239:TRP:HB2	1:B:247:ARG:HB2	1.71	0.73
1:J:285:ASN:HD22	1:J:288:LEU:N	1.87	0.73
1:I:36:LYS:HG3	6:I:1064:HOH:O	1.89	0.72
1:Q:126:LYS:HB2	1:Q:358:ARG:HD2	1.70	0.72
1:Q:188:THR:HG22	1:Q:223:PRO:HG2	1.72	0.72
1:R:308:LEU:HD13	1:R:310:LEU:HD11	1.71	0.72
1:J:143:ARG:HG2	1:J:144:CYS:N	2.04	0.72
1:P:285:ASN:HB2	1:P:291:ILE:HD11	1.71	0.72
1:G:285:ASN:HD22	1:G:287:ARG:N	1.87	0.72
1:L:166:GLU:HG3	1:L:184:TYR:OH	1.89	0.72
1:H:297:ASN:HB3	1:H:301:VAL:HG13	1.72	0.72
1:N:57:VAL:HG22	1:N:63:THR:HG22	1.70	0.72
1:O:325:LYS:HD3	1:O:389:PRO:HB2	1.70	0.72
1:C:108:ILE:HG21	1:C:296:THR:HG22	1.70	0.72
1:F:137:VAL:HG13	1:F:306:VAL:HB	1.70	0.72
1:M:50:TYR:O	1:M:54:TRP:HB3	1.89	0.71
1:P:202:HIS:HB3	3:P:616:ADP:H1'	1.71	0.71
1:O:278:CYS:HB3	1:O:280:HIS:CE1	2.26	0.71
1:E:140:CYS:HB2	1:E:260:VAL:HG21	1.71	0.71
1:E:239:TRP:HB2	1:E:247:ARG:HB2	1.72	0.71
1:Q:143:ARG:HG2	1:Q:144:CYS:N	2.04	0.71
1:F:253:LYS:HE3	6:F:1023:HOH:O	1.90	0.70

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:346:ASP:HB2	6:E:2939:HOH:O	1.90	0.70
1:L:313:LEU:O	1:L:313:LEU:HD23	1.91	0.70
1:I:201:ASP:HB3	1:I:203:PHE:CE2	2.25	0.70
1:O:168:VAL:HG13	1:O:280:HIS:CE1	2.26	0.70
1:R:41:MET:HE2	1:R:71:GLY:HA3	1.72	0.70
1:C:309:ARG:NH1	1:C:342:ASP:OD1	2.23	0.70
1:C:313:LEU:CD1	1:C:374:CYS:HB3	2.22	0.70
1:H:372:ILE:HG22	1:H:376:LYS:HE2	1.74	0.70
1:J:292:CYS:HB2	1:J:297:ASN:O	1.92	0.70
1:N:297:ASN:HB3	1:N:301:VAL:HG13	1.72	0.69
1:J:28:ALA:HB2	6:J:2425:HOH:O	1.92	0.69
1:K:188:THR:HG22	1:K:223:PRO:HG2	1.73	0.69
1:H:143:ARG:HG2	1:H:144:CYS:N	2.08	0.69
1:I:385:ASP:HB2	1:Q:134:ASP:OD2	1.92	0.69
1:L:60:ASN:HD22	1:L:90:ASP:HB2	1.58	0.69
1:P:143:ARG:HG2	1:P:144:CYS:N	2.07	0.69
1:H:352:ARG:CG	1:H:352:ARG:HH11	2.06	0.69
1:D:8:TYR:HD2	1:D:11:LYS:HZ3	1.39	0.69
1:H:134:ASP:HB2	6:H:3034:HOH:O	1.93	0.68
1:C:143:ARG:HD3	1:C:303:ARG:HB3	1.75	0.68
1:F:155:PRO:HB3	1:F:216:SER:O	1.94	0.68
1:L:162:ARG:HD3	1:L:226:ARG:HD2	1.74	0.68
1:Q:236:PHE:CE1	1:Q:267:GLY:HA3	2.29	0.68
1:O:91:GLU:OE2	1:O:149:LYS:HE2	1.93	0.68
1:O:50:TYR:O	1:O:54:TRP:HB3	1.94	0.68
1:F:331:ARG:HG2	1:F:336:GLU:HA	1.75	0.68
1:G:168:VAL:HG13	1:G:280:HIS:CE1	2.29	0.68
1:K:94:TYR:CZ	1:K:288:LEU:HD11	2.29	0.68
1:B:66:LYS:O	1:B:66:LYS:HD3	1.93	0.68
1:O:195:GLN:O	1:O:199:ILE:HG13	1.93	0.68
1:N:128:VAL:HG11	1:O:358:ARG:NH2	2.08	0.68
1:N:285:ASN:HD22	1:N:288:LEU:N	1.90	0.68
1:D:297:ASN:HB3	1:D:301:VAL:HG13	1.76	0.67
1:B:247:ARG:NH1	3:B:602:ADP:O1B	2.25	0.67
1:I:384:ILE:HA	1:I:387:MET:HG3	1.76	0.67
1:N:168:VAL:O	1:N:171:ASP:HB2	1.93	0.67
1:N:117:HIS:ND1	1:N:353:LEU:HD23	2.10	0.67
1:B:166:GLU:OE1	1:B:225:GLY:HA2	1.94	0.67
1:D:239:TRP:HB2	1:D:247:ARG:HB2	1.74	0.67
1:E:287:ARG:HD3	6:E:1863:HOH:O	1.95	0.67
1:O:68:ILE:O	1:O:72:VAL:HG23	1.95	0.67
1:G:328:LEU:HD11	1:G:367:GLY:HA3	1.76	0.67

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:98:LYS:HE3	1:D:102:ASP:OD2	1.95	0.67
1:L:41:MET:HE2	1:L:71:GLY:HA3	1.77	0.67
1:C:54:TRP:HZ3	6:C:2582:HOH:O	1.76	0.66
1:L:361:VAL:O	1:L:365:VAL:HG23	1.95	0.66
1:M:285:ASN:HD22	1:M:287:ARG:H	1.43	0.66
1:E:323:LEU:HD21	1:E:347:ILE:HD12	1.78	0.66
1:R:239:TRP:HB2	1:R:247:ARG:HB2	1.76	0.66
3:L:612:ADP:O2B	3:L:612:ADP:H5'2	1.96	0.66
1:M:38:ASN:ND2	1:M:82:LYS:HE3	2.11	0.66
1:Q:36:LYS:HE3	6:Q:2740:HOH:O	1.95	0.66
1:G:152:CYS:SG	1:H:17:SER:HB3	2.35	0.66
1:K:191:ASN:ND2	1:K:193:LYS:HB2	2.08	0.65
1:L:230:HIS:ND1	1:L:234:LYS:HG3	2.12	0.65
1:C:285:ASN:HD22	1:C:288:LEU:H	1.45	0.65
1:B:302:VAL:O	1:B:352:ARG:HD3	1.95	0.65
1:D:322:MET:HG3	1:D:389:PRO:HD2	1.79	0.65
1:K:244:ASP:OD1	1:K:292:CYS:HB3	1.97	0.65
1:O:357:GLU:O	1:O:361:VAL:HG23	1.97	0.65
1:N:285:ASN:ND2	1:N:288:LEU:H	1.92	0.65
1:Q:143:ARG:HG3	6:Q:1134:HOH:O	1.96	0.65
1:N:239:TRP:HB2	1:N:247:ARG:HB2	1.78	0.65
1:K:141:ARG:HG3	1:K:251:MET:HB3	1.76	0.65
1:D:252:GLN:NE2	1:D:256:ASP:HB3	2.12	0.65
1:J:146:ARG:HD2	1:J:282:LEU:HD13	1.79	0.65
1:J:191:ASN:HB2	6:Q:1062:HOH:O	1.97	0.65
1:D:123:ASP:OD1	1:D:125:ASN:HB2	1.96	0.65
1:N:357:GLU:O	1:N:361:VAL:HG23	1.96	0.65
1:L:143:ARG:HG2	1:L:144:CYS:N	2.12	0.65
1:G:36:LYS:HG3	6:G:3265:HOH:O	1.97	0.65
1:E:298:MET:CE	1:E:353:LEU:HD12	2.27	0.65
1:R:305:SER:HB3	1:R:348:SER:HB3	1.79	0.65
1:P:192:GLU:O	1:P:196:GLU:HG3	1.97	0.64
1:C:304:ALA:O	1:C:348:SER:HB2	1.97	0.64
1:D:199:ILE:HD13	1:D:206:GLU:HA	1.79	0.64
1:A:352:ARG:HG2	1:A:352:ARG:HH11	1.62	0.64
1:L:26:LYS:O	1:L:29:ASP:HB2	1.97	0.64
1:G:357:GLU:O	1:G:361:VAL:HG23	1.97	0.64
1:R:205:PHE:CG	1:R:242:GLU:HG3	2.33	0.64
1:Q:285:ASN:HD22	1:Q:288:LEU:N	1.96	0.64
1:O:98:LYS:HE3	1:O:102:ASP:OD2	1.96	0.64
1:D:49:LEU:HD21	1:D:99:GLU:HG2	1.78	0.64
1:B:312:PHE:CZ	1:B:379:GLU:HG3	2.32	0.64

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:143:ARG:NH1	3:D:604:ADP:O3B	2.30	0.64
1:E:180:LEU:O	1:E:229:TRP:HH2	1.81	0.64
1:H:177:LYS:HB3	6:H:2402:HOH:O	1.95	0.64
1:C:44:GLN:OE1	1:C:103:LYS:HB3	1.98	0.64
1:D:256:ASP:OD2	1:D:259:ALA:HB2	1.97	0.64
1:I:57:VAL:HG11	1:I:61:GLY:HA2	1.79	0.64
1:L:257:LEU:HD11	1:L:364:LEU:HD13	1.79	0.64
1:R:359:GLU:O	1:R:363:VAL:HG23	1.97	0.64
1:B:105:ILE:HG23	1:B:298:MET:HE1	1.79	0.64
1:Q:40:VAL:HG12	1:Q:104:CYS:SG	2.37	0.64
1:R:210:GLY:HA3	6:R:2262:HOH:O	1.97	0.64
1:L:60:ASN:HD22	1:L:90:ASP:CB	2.11	0.64
1:I:57:VAL:CG1	1:I:61:GLY:HA2	2.28	0.64
1:D:284:HIS:CE1	1:D:289:GLY:HA2	2.32	0.64
1:O:336:GLU:OE2	2:O:515:NMG:NE	2.29	0.64
1:Q:285:ASN:HB2	1:Q:291:ILE:HD11	1.80	0.64
1:R:205:PHE:CD1	1:R:242:GLU:HG3	2.33	0.64
1:J:318:ARG:HD3	1:J:388:ILE:HD12	1.80	0.64
1:G:180:LEU:O	1:G:229:TRP:HH2	1.81	0.64
1:Q:285:ASN:HB3	1:Q:288:LEU:HB2	1.80	0.64
1:K:38:ASN:ND2	1:K:82:LYS:HG3	2.13	0.63
1:A:213:LEU:HD12	1:A:218:CYS:HB2	1.79	0.63
1:K:132:PHE:HZ	1:K:365:VAL:HG22	1.63	0.63
1:A:108:ILE:HG21	1:A:296:THR:HG22	1.81	0.63
1:I:191:ASN:HD21	1:I:193:LYS:HB2	1.61	0.63
1:D:109:HIS:O	1:D:110:HIS:HB2	1.98	0.63
1:G:121:ASP:OD2	1:G:358:ARG:HD3	1.97	0.63
1:G:384:ILE:HA	1:G:387:MET:HG3	1.78	0.63
1:F:219:ALA:O	1:F:222:TRP:HB2	1.97	0.63
1:I:385:ASP:HB2	1:Q:134:ASP:CG	2.19	0.63
1:F:152:CYS:HB2	1:F:161:GLU:OE1	1.99	0.63
1:L:274:LEU:HB3	6:L:3192:HOH:O	1.99	0.63
1:H:314:GLU:HG3	1:H:315:LYS:HD2	1.80	0.63
1:M:168:VAL:HG13	1:M:280:HIS:CE1	2.34	0.63
1:O:38:ASN:HD22	1:O:38:ASN:C	2.02	0.63
1:Q:326:LEU:HD11	1:Q:370:LEU:HD23	1.80	0.63
1:O:303:ARG:NE	3:O:615:ADP:O3B	2.28	0.63
1:C:378:LEU:HD21	1:C:384:ILE:HG12	1.81	0.62
1:D:142:ILE:HD11	1:D:257:LEU:CD2	2.29	0.62
1:I:183:LYS:HD3	1:I:185:TYR:CE2	2.34	0.62
1:Q:314:GLU:HG3	1:Q:315:LYS:HD2	1.81	0.62
1:G:39:ASN:HB2	1:G:83:LYS:O	1.99	0.62

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:250:SER:HB3	1:F:264:PHE:HB2	1.79	0.62
1:R:20:TRP:HA	1:R:54:TRP:CH2	2.34	0.62
1:H:106:GLU:OE2	1:H:112:LYS:HG2	2.00	0.62
1:P:105:ILE:HG12	1:P:298:MET:HE3	1.82	0.62
1:P:140:CYS:HB2	1:P:260:VAL:HG21	1.80	0.62
1:J:154:PRO:HD3	1:J:245:HIS:CD2	2.34	0.62
2:B:502:NMG:NH1	5:B:802:NO3:N	2.48	0.62
1:D:153:LEU:HD21	1:D:283:MET:HE3	1.81	0.62
1:R:142:ILE:HG13	1:R:260:VAL:HG12	1.81	0.62
1:N:176:LEU:HD13	1:N:229:TRP:CH2	2.34	0.62
1:M:32:PRO:HD3	1:N:159:ARG:NH2	2.15	0.62
1:G:317:PRO:HB2	1:O:253:LYS:HD2	1.80	0.62
1:L:314:GLU:HG3	1:L:315:LYS:HD2	1.81	0.62
1:G:154:PRO:HG2	1:G:243:GLU:O	1.99	0.62
1:K:102:ASP:OD2	1:K:113:PRO:HB3	1.99	0.62
1:N:189:THR:HG21	6:N:2920:HOH:O	1.99	0.62
1:J:357:GLU:O	1:J:361:VAL:HG23	2.00	0.62
1:J:297:ASN:HB3	1:J:301:VAL:HG13	1.82	0.61
1:H:159:ARG:NH1	1:H:221:ASP:OD1	2.31	0.61
1:P:49:LEU:HD21	1:P:99:GLU:HG2	1.82	0.61
1:K:285:ASN:HD22	1:K:287:ARG:N	1.98	0.61
1:N:231:ASN:OD1	1:N:234:LYS:N	2.32	0.61
1:L:98:LYS:HE3	1:L:102:ASP:OD2	2.00	0.61
1:A:52:LYS:HE2	1:A:53:TYR:CE2	2.36	0.61
1:P:38:ASN:HA	6:P:1820:HOH:O	2.01	0.61
1:J:183:LYS:HD3	1:J:185:TYR:CZ	2.35	0.61
1:A:24:LYS:HG3	1:A:25:PHE:H	1.66	0.61
1:K:126:LYS:HB2	1:K:358:ARG:HD2	1.81	0.61
1:K:226:ARG:HG3	1:K:241:ASN:O	2.01	0.61
1:B:39:ASN:OD1	1:B:41:MET:HB3	2.00	0.61
1:F:331:ARG:HB2	1:F:346:ASP:HB3	1.83	0.61
1:D:252:GLN:HE22	1:D:256:ASP:HB3	1.66	0.61
1:G:143:ARG:HG2	1:G:144:CYS:N	2.15	0.61
1:I:141:ARG:HG3	1:I:251:MET:HB3	1.81	0.61
1:A:295:PRO:O	1:A:298:MET:HG3	2.00	0.61
1:C:50:TYR:O	1:C:54:TRP:HB3	2.01	0.61
1:C:385:ASP:HA	1:C:388:ILE:HD12	1.83	0.61
1:C:192:GLU:O	1:C:196:GLU:HG3	2.00	0.61
1:A:192:GLU:HG2	1:A:196:GLU:OE2	2.01	0.61
1:L:281:GLY:O	1:L:282:LEU:HD23	2.00	0.60
1:F:244:ASP:OD1	1:F:292:CYS:HB3	2.01	0.60
1:F:143:ARG:HD3	1:F:303:ARG:HB3	1.82	0.60

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:H:270:GLU:OE1	1:H:273:ARG:NH1	2.34	0.60
1:O:188:THR:HG23	6:O:1195:HOH:O	2.02	0.60
1:G:285:ASN:HD22	1:G:286:ASP:N	1.99	0.60
1:H:312:PHE:HB2	1:H:375:ASP:OD1	2.00	0.60
1:A:238:VAL:HA	1:A:247:ARG:O	2.01	0.60
1:N:146:ARG:HB3	1:N:282:LEU:HD22	1.83	0.60
1:I:95:GLU:HG3	6:I:1517:HOH:O	2.02	0.60
1:L:188:THR:CG2	1:L:223:PRO:HG2	2.30	0.60
1:P:18:LYS:O	1:P:21:GLU:HG2	2.02	0.60
1:K:285:ASN:ND2	1:K:287:ARG:H	2.00	0.60
1:E:144:CYS:HB3	1:E:302:VAL:HG22	1.82	0.60
1:K:158:SER:OG	1:K:161:GLU:HG3	2.01	0.60
1:P:285:ASN:HD22	1:P:288:LEU:H	1.50	0.60
1:F:202:HIS:HB3	3:F:606:ADP:H1'	1.82	0.60
1:G:142:ILE:HG22	1:G:264:PHE:CD1	2.37	0.60
1:H:364:LEU:HD22	1:H:368:VAL:HG23	1.83	0.60
1:J:240:ILE:O	1:J:241:ASN:HB2	2.01	0.60
1:R:314:GLU:HB2	1:R:345:TYR:OH	2.00	0.60
1:L:147:SER:HA	1:L:245:HIS:HB2	1.84	0.60
1:I:297:ASN:HB3	1:I:301:VAL:HG13	1.84	0.60
1:L:27:ALA:HB3	1:L:51:GLU:HG2	1.83	0.60
1:L:108:ILE:HD13	1:L:296:THR:HG22	1.84	0.60
1:J:314:GLU:HG3	1:J:315:LYS:HD2	1.83	0.60
1:D:49:LEU:HD11	1:D:103:LYS:HE2	1.82	0.60
1:G:184:TYR:OH	1:G:227:GLY:HA3	2.02	0.60
1:C:98:LYS:HG3	1:C:102:ASP:OD2	2.02	0.60
1:I:143:ARG:HG2	1:I:144:CYS:N	2.16	0.60
1:G:168:VAL:HG13	1:G:280:HIS:ND1	2.16	0.60
1:H:308:LEU:HD13	1:H:310:LEU:HD21	1.84	0.60
1:K:313:LEU:HD23	1:K:313:LEU:O	2.02	0.60
1:Q:153:LEU:HD21	1:Q:283:MET:SD	2.42	0.60
1:I:247:ARG:NH1	3:I:609:ADP:O1B	2.35	0.60
1:D:105:ILE:HG12	1:D:298:MET:HE2	1.84	0.59
1:F:296:THR:O	1:F:352:ARG:HD2	2.02	0.59
1:B:117:HIS:ND1	1:B:118:PRO:HD2	2.16	0.59
1:P:294:CYS:SG	1:P:296:THR:HG23	2.42	0.59
1:D:143:ARG:HD3	1:D:303:ARG:HB3	1.84	0.59
1:F:31:PHE:CE2	1:F:47:LYS:HE3	2.38	0.59
1:R:192:GLU:O	1:R:196:GLU:HG3	2.02	0.59
1:M:53:TYR:CZ	1:M:97:TYR:HA	2.38	0.59
1:Q:168:VAL:HG13	1:Q:280:HIS:CE1	2.38	0.59
1:J:187:LEU:HB3	1:J:223:PRO:HB2	1.84	0.59

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:Q:84:THR:HG22	1:Q:86:CYS:SG	2.43	0.59
1:A:44:GLN:NE2	1:A:107:GLU:OE1	2.35	0.59
1:D:105:ILE:HG12	1:D:298:MET:CE	2.33	0.59
1:E:151:VAL:CG1	1:E:152:CYS:N	2.65	0.59
1:F:143:ARG:HG2	1:F:144:CYS:N	2.17	0.59
1:I:312:PHE:HB2	1:I:375:ASP:OD1	2.02	0.59
1:I:49:LEU:HD21	1:I:99:GLU:HG2	1.85	0.59
1:P:331:ARG:HB2	1:P:346:ASP:HB3	1.84	0.59
1:O:385:ASP:HB2	6:O:1252:HOH:O	2.01	0.59
1:E:252:GLN:OE1	1:E:263:ARG:NH2	2.30	0.59
1:O:361:VAL:O	1:O:365:VAL:HG23	2.03	0.59
1:K:298:MET:HG2	6:K:1698:HOH:O	2.02	0.59
1:C:364:LEU:HD22	1:C:368:VAL:HG23	1.84	0.59
1:I:104:CYS:O	1:I:108:ILE:HG13	2.03	0.59
1:D:31:PHE:CD1	1:D:32:PRO:HD2	2.38	0.58
1:I:308:LEU:O	1:I:344:THR:HA	2.03	0.58
1:F:298:MET:CE	1:F:353:LEU:HD12	2.33	0.58
1:F:123:ASP:OD2	1:F:126:LYS:HG2	2.02	0.58
1:G:268:LEU:O	1:G:272:GLU:HG3	2.03	0.58
1:D:90:ASP:HB2	6:D:1569:HOH:O	2.03	0.58
1:F:191:ASN:HD21	1:F:193:LYS:HB2	1.68	0.58
1:D:313:LEU:O	1:D:313:LEU:HD23	2.03	0.58
1:H:322:MET:HG3	1:H:389:PRO:HD2	1.84	0.58
1:C:27:ALA:HB2	1:C:54:TRP:CD1	2.38	0.58
1:J:206:GLU:HG2	6:J:1216:HOH:O	2.03	0.58
1:B:374:CYS:O	1:B:378:LEU:HG	2.04	0.58
1:A:288:LEU:HD22	1:A:353:LEU:HD11	1.86	0.58
1:N:59:PRO:HG2	1:N:92:TYR:CE2	2.39	0.58
1:I:250:SER:HB3	1:I:264:PHE:HB2	1.84	0.58
1:B:53:TYR:HB3	1:B:97:TYR:HD2	1.69	0.58
1:N:144:CYS:HA	1:N:301:VAL:O	2.03	0.58
1:E:105:ILE:HG12	1:E:298:MET:CE	2.33	0.58
1:A:104:CYS:O	1:A:108:ILE:HG13	2.03	0.58
1:D:60:ASN:HB2	1:D:90:ASP:OD2	2.04	0.58
1:Q:149:LYS:HB3	1:Q:281:GLY:O	2.02	0.58
1:C:144:CYS:HA	1:C:301:VAL:O	2.03	0.58
1:D:201:ASP:HB3	1:D:203:PHE:CE2	2.38	0.58
1:I:318:ARG:HA	6:I:2048:HOH:O	2.04	0.58
1:A:236:PHE:CZ	1:A:267:GLY:HA3	2.38	0.58
1:I:151:VAL:HG12	1:I:152:CYS:N	2.19	0.58
1:R:154:PRO:HG2	1:R:243:GLU:O	2.04	0.58
1:N:300:THR:HB	1:N:302:VAL:HG23	1.86	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:K:285:ASN:HD22	1:K:287:ARG:H	1.52	0.58
1:O:112:LYS:HG3	6:O:3305:HOH:O	2.02	0.58
1:H:331:ARG:HB2	1:H:346:ASP:HB3	1.85	0.58
1:B:183:LYS:HD3	1:B:185:TYR:CE2	2.39	0.58
1:C:367:GLY:O	1:C:371:LEU:HG	2.04	0.58
1:E:173:LEU:HD13	1:E:229:TRP:CG	2.38	0.58
1:K:113:PRO:HD3	6:K:1628:HOH:O	2.04	0.58
1:P:124:HIS:O	1:P:258:LYS:HE3	2.04	0.58
1:M:244:ASP:OD1	1:M:292:CYS:HB3	2.04	0.58
1:D:142:ILE:HD11	1:D:257:LEU:HD23	1.85	0.57
1:H:184:TYR:CD2	1:H:186:PRO:HD3	2.39	0.57
1:R:384:ILE:HA	1:R:387:MET:HG3	1.86	0.57
1:Q:223:PRO:HD2	6:Q:1534:HOH:O	2.05	0.57
1:A:154:PRO:N	1:A:155:PRO:HD2	2.19	0.57
1:P:319:PHE:HB3	6:P:1899:HOH:O	2.03	0.57
1:E:208:PRO:HG3	1:E:222:TRP:CD2	2.38	0.57
3:D:604:ADP:H2'	6:D:1076:HOH:O	2.04	0.57
1:K:144:CYS:HG	1:K:264:PHE:HZ	1.51	0.57
1:G:37:HIS:CD2	1:G:75:PRO:HA	2.39	0.57
1:K:38:ASN:HD22	1:K:38:ASN:C	2.07	0.57
1:N:94:TYR:HE2	1:N:102:ASP:OD1	1.86	0.57
1:E:141:ARG:NH1	3:E:605:ADP:O2B	2.37	0.57
1:L:60:ASN:ND2	1:L:90:ASP:HB2	2.19	0.57
1:L:252:GLN:OE1	1:L:263:ARG:NH2	2.38	0.57
1:B:331:ARG:HB2	1:B:346:ASP:HB3	1.86	0.57
1:F:94:TYR:CZ	1:F:288:LEU:HD11	2.40	0.57
1:H:285:ASN:ND2	1:H:287:ARG:H	2.02	0.57
1:D:298:MET:HG2	6:D:2110:HOH:O	2.04	0.57
1:A:201:ASP:O	1:A:202:HIS:HB2	2.04	0.57
1:N:94:TYR:CZ	1:N:288:LEU:HD11	2.39	0.57
1:E:298:MET:HE3	1:E:353:LEU:HD12	1.85	0.57
1:R:106:GLU:OE2	1:R:112:LYS:HE2	2.05	0.57
1:L:161:GLU:O	1:L:165:VAL:HG23	2.05	0.56
1:N:188:THR:HG23	6:N:1355:HOH:O	2.04	0.56
1:G:202:HIS:HB3	3:G:607:ADP:H1'	1.87	0.56
1:K:144:CYS:HA	1:K:301:VAL:O	2.04	0.56
1:L:252:GLN:HB2	6:L:2314:HOH:O	2.05	0.56
1:A:152:CYS:SG	1:B:17:SER:HB3	2.45	0.56
1:N:18:LYS:O	1:N:21:GLU:HG2	2.05	0.56
1:C:372:ILE:HG22	1:C:376:LYS:HE2	1.87	0.56
1:G:313:LEU:HD23	1:G:313:LEU:O	2.06	0.56
1:D:33:ASP:C	1:D:34:LEU:HD23	2.26	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:318:ARG:HD3	1:E:388:ILE:HD13	1.87	0.56
1:R:285:ASN:HD22	1:R:288:LEU:HB2	1.68	0.56
1:Q:288:LEU:O	1:Q:299:GLY:HA2	2.06	0.56
1:N:245:HIS:O	1:N:246:ILE:HG13	2.04	0.56
1:F:303:ARG:NE	3:F:606:ADP:O3B	2.33	0.56
1:F:191:ASN:ND2	1:F:193:LYS:H	2.02	0.56
1:B:183:LYS:HG2	1:B:184:TYR:N	2.21	0.56
1:A:357:GLU:O	1:A:361:VAL:HG23	2.04	0.56
1:L:18:LYS:O	1:L:21:GLU:HG2	2.06	0.56
1:L:187:LEU:HD11	1:L:195:GLN:NE2	2.21	0.56
1:G:297:ASN:HB3	1:G:301:VAL:HG13	1.86	0.56
1:R:12:ASN:HA	6:R:3065:HOH:O	2.04	0.56
1:D:39:ASN:HA	1:D:82:LYS:HE2	1.87	0.56
1:F:304:ALA:O	1:F:348:SER:HB2	2.06	0.56
1:F:157:MET:HA	1:F:161:GLU:OE1	2.05	0.56
1:K:297:ASN:HB3	1:K:301:VAL:HG13	1.88	0.56
1:C:69:GLN:NE2	1:C:73:ASP:OD1	2.37	0.56
1:B:84:THR:HG23	1:B:108:ILE:HD11	1.86	0.56
1:E:297:ASN:HB3	1:E:301:VAL:HG13	1.88	0.56
1:L:144:CYS:HB3	1:L:302:VAL:HG22	1.88	0.56
1:P:314:GLU:HG3	1:P:315:LYS:HD2	1.88	0.56
1:A:38:ASN:ND2	6:A:1164:HOH:O	2.38	0.56
1:O:147:SER:O	1:O:282:LEU:HA	2.06	0.56
1:Q:352:ARG:HG2	1:Q:352:ARG:HH11	1.71	0.56
1:A:313:LEU:HD22	1:A:319:PHE:CD1	2.41	0.55
1:C:127:LEU:HD23	1:C:258:LYS:HG3	1.87	0.55
1:L:229:TRP:O	1:L:229:TRP:HE3	1.88	0.55
1:N:108:ILE:HG21	1:N:296:THR:HG22	1.88	0.55
1:L:313:LEU:HD12	1:L:374:CYS:HB2	1.88	0.55
1:D:132:PHE:HE1	1:D:257:LEU:HD12	1.72	0.55
1:R:243:GLU:HB3	6:R:1914:HOH:O	2.05	0.55
1:M:359:GLU:O	1:M:363:VAL:HG23	2.07	0.55
1:M:313:LEU:HD23	1:M:313:LEU:O	2.06	0.55
1:E:331:ARG:HB2	1:E:346:ASP:HB3	1.88	0.55
1:L:238:VAL:HG22	1:L:248:VAL:HA	1.88	0.55
1:R:113:PRO:HA	1:R:287:ARG:NH2	2.21	0.55
1:J:180:LEU:O	1:J:229:TRP:HH2	1.89	0.55
1:L:305:SER:HB2	1:L:348:SER:HB3	1.87	0.55
1:F:305:SER:CB	1:F:348:SER:HB3	2.31	0.55
1:C:292:CYS:SG	1:C:301:VAL:HG11	2.46	0.55
1:F:233:GLU:HG3	6:F:3273:HOH:O	2.05	0.55
1:C:105:ILE:HG12	1:C:298:MET:CE	2.36	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:M:121:ASP:OD2	1:M:358:ARG:HD3	2.05	0.55
1:D:285:ASN:ND2	1:D:288:LEU:H	1.87	0.55
1:Q:247:ARG:NH1	3:Q:617:ADP:O1B	2.36	0.55
1:I:384:ILE:CA	1:I:387:MET:HG3	2.36	0.55
1:H:111:PHE:CG	1:H:353:LEU:HD13	2.40	0.55
1:N:359:GLU:O	1:N:363:VAL:HG23	2.07	0.55
1:I:142:ILE:HD11	1:I:257:LEU:CD2	2.37	0.55
1:F:298:MET:HE3	1:F:353:LEU:HD12	1.89	0.55
1:B:59:PRO:HD2	1:B:92:TYR:CD1	2.42	0.55
1:D:267:GLY:O	1:D:271:VAL:HG23	2.06	0.55
1:J:112:LYS:O	1:J:115:ASP:HB2	2.07	0.55
1:I:152:CYS:SG	1:J:17:SER:HB3	2.47	0.55
1:Q:357:GLU:O	1:Q:361:VAL:HG23	2.06	0.55
1:E:314:GLU:HG2	1:E:315:LYS:HD2	1.87	0.55
1:N:285:ASN:HB2	1:N:291:ILE:HD11	1.89	0.55
1:H:239:TRP:HB2	1:H:247:ARG:HB2	1.88	0.55
1:B:146:ARG:HB3	1:B:282:LEU:HD22	1.89	0.55
1:G:285:ASN:ND2	1:G:286:ASP:N	2.55	0.55
1:G:34:LEU:HA	1:G:37:HIS:ND1	2.22	0.55
1:F:59:PRO:HD2	1:F:92:TYR:CD1	2.42	0.55
1:H:136:TYR:HE2	1:H:375:ASP:OD2	1.90	0.54
1:J:192:GLU:O	1:J:196:GLU:HG3	2.08	0.54
1:H:223:PRO:HD2	6:H:1907:HOH:O	2.06	0.54
1:N:235:ASN:HB2	1:N:263:ARG:NH1	2.23	0.54
1:N:34:LEU:HA	1:N:37:HIS:ND1	2.21	0.54
1:L:127:LEU:HD12	1:L:362:GLN:OE1	2.07	0.54
1:F:230:HIS:HB3	1:F:237:LEU:HD23	1.88	0.54
1:A:34:LEU:HA	1:A:37:HIS:ND1	2.21	0.54
1:P:270:GLU:OE2	1:P:270:GLU:HA	2.06	0.54
1:Q:148:VAL:HG12	1:Q:148:VAL:O	2.06	0.54
1:E:252:GLN:HG2	1:E:260:VAL:HG22	1.88	0.54
1:N:246:ILE:O	1:N:247:ARG:HG2	2.07	0.54
1:E:296:THR:O	1:E:352:ARG:HG3	2.07	0.54
1:E:205:PHE:HB2	1:E:242:GLU:OE2	2.06	0.54
1:N:143:ARG:HG2	1:N:144:CYS:N	2.21	0.54
1:K:285:ASN:HD22	1:K:288:LEU:H	1.55	0.54
1:O:127:LEU:HD12	1:O:362:GLN:OE1	2.08	0.54
1:F:37:HIS:O	1:K:177:LYS:HB3	2.07	0.54
1:H:352:ARG:NH1	1:H:352:ARG:CG	2.70	0.54
1:M:310:LEU:HD13	1:M:313:LEU:HD22	1.90	0.54
1:A:143:ARG:HG2	1:A:144:CYS:N	2.22	0.54
1:R:34:LEU:HA	1:R:37:HIS:ND1	2.22	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:I:39:ASN:HB2	1:I:83:LYS:O	2.06	0.54
1:R:188:THR:CG2	1:R:223:PRO:HG2	2.37	0.54
1:D:143:ARG:NH1	1:D:303:ARG:HD3	2.23	0.54
1:A:251:MET:O	1:A:252:GLN:HB3	2.08	0.54
1:N:205:PHE:CG	1:N:242:GLU:HG3	2.42	0.54
1:D:70:THR:HG22	6:D:2528:HOH:O	2.08	0.54
1:P:13:ARG:HG2	6:P:1900:HOH:O	2.08	0.54
1:N:247:ARG:NH1	3:N:614:ADP:O1B	2.41	0.54
1:G:205:PHE:HD2	1:G:239:TRP:CD2	2.25	0.54
1:A:122:LEU:HD12	1:A:269:LEU:HD21	1.89	0.54
1:Q:37:HIS:CD2	1:Q:75:PRO:HA	2.43	0.54
1:D:314:GLU:HG3	1:D:315:LYS:HD2	1.89	0.54
1:C:302:VAL:O	1:C:352:ARG:HD3	2.06	0.54
1:M:302:VAL:O	1:M:352:ARG:HD3	2.06	0.54
1:G:185:TYR:N	1:G:185:TYR:CD1	2.76	0.54
1:H:352:ARG:HG2	1:H:352:ARG:HH11	1.72	0.54
1:H:207:LYS:O	1:H:209:THR:N	2.35	0.54
1:J:372:ILE:HG22	1:J:376:LYS:HE2	1.89	0.54
1:K:66:LYS:HG3	1:L:15:GLY:O	2.08	0.54
1:K:340:ALA:HB2	1:K:345:TYR:CE2	2.42	0.54
1:B:53:TYR:HB3	1:B:97:TYR:CD2	2.43	0.54
1:K:34:LEU:HD21	1:K:72:VAL:HG22	1.89	0.54
1:A:67:CYS:O	1:A:86:CYS:HA	2.07	0.54
1:I:285:ASN:ND2	1:I:287:ARG:H	2.05	0.54
1:A:201:ASP:HB3	1:A:203:PHE:CE2	2.42	0.54
1:E:220:ARG:HG2	1:F:69:GLN:NE2	2.22	0.54
1:O:359:GLU:O	1:O:363:VAL:HG23	2.08	0.54
1:M:57:VAL:CG1	1:M:61:GLY:HA2	2.38	0.54
1:R:313:LEU:HD23	1:R:316:HIS:HB3	1.90	0.54
1:M:191:ASN:HD21	1:M:193:LYS:HB2	1.72	0.53
1:F:18:LYS:O	1:F:21:GLU:HG2	2.08	0.53
1:H:364:LEU:HD22	1:H:368:VAL:CG2	2.38	0.53
1:B:183:LYS:HD3	1:B:185:TYR:CZ	2.43	0.53
1:O:53:TYR:OH	1:O:99:GLU:HB3	2.08	0.53
1:P:109:HIS:O	1:P:110:HIS:HB2	2.07	0.53
1:Q:110:HIS:CD2	1:Q:327:ARG:CZ	2.91	0.53
1:C:66:LYS:HE3	1:D:16:HIS:CD2	2.44	0.53
1:L:346:ASP:O	1:L:346:ASP:OD1	2.26	0.53
1:I:94:TYR:CE1	1:I:288:LEU:HD11	2.43	0.53
1:G:331:ARG:HB2	1:G:346:ASP:CB	2.38	0.53
1:R:308:LEU:HD13	1:R:310:LEU:CD1	2.38	0.53
1:J:50:TYR:O	1:J:54:TRP:HB3	2.08	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:217:GLY:HA2	6:G:1338:HOH:O	2.07	0.53
1:I:147:SER:O	1:I:282:LEU:HA	2.09	0.53
1:H:189:THR:O	1:P:36:LYS:HG2	2.09	0.53
1:C:361:VAL:O	1:C:365:VAL:HG23	2.07	0.53
1:N:296:THR:O	1:N:352:ARG:HG3	2.08	0.53
1:N:187:LEU:HB3	1:N:223:PRO:HB2	1.90	0.53
1:K:142:ILE:HD12	1:K:260:VAL:HG12	1.89	0.53
3:R:618:ADP:O1B	5:R:818:NO3:N	2.42	0.53
1:C:109:HIS:O	1:C:110:HIS:HB2	2.08	0.53
1:N:285:ASN:HD22	1:N:288:LEU:HG	1.70	0.53
1:N:128:VAL:HG11	1:O:358:ARG:HH21	1.72	0.53
1:G:83:LYS:NZ	6:G:1095:HOH:O	2.40	0.53
1:K:313:LEU:HD22	1:K:319:PHE:CD1	2.43	0.53
1:D:105:ILE:HG23	1:D:298:MET:HE1	1.91	0.53
1:E:151:VAL:HG13	1:E:152:CYS:N	2.24	0.53
1:A:384:ILE:O	1:A:388:ILE:HG13	2.08	0.53
1:D:195:GLN:O	1:D:199:ILE:HG13	2.08	0.53
1:G:239:TRP:HB2	1:G:247:ARG:HB2	1.90	0.53
1:D:213:LEU:O	1:D:213:LEU:HG	2.09	0.53
1:B:121:ASP:O	1:B:357:GLU:HB2	2.09	0.53
1:R:314:GLU:CG	1:R:315:LYS:HD2	2.38	0.53
1:O:56:LYS:NZ	1:O:96:CYS:HA	2.24	0.53
1:F:197:GLN:NE2	1:F:200:GLU:OE1	2.41	0.53
1:I:142:ILE:HD12	1:I:260:VAL:HG12	1.91	0.53
1:N:105:ILE:HG12	1:N:298:MET:HE1	1.91	0.53
1:O:236:PHE:CE1	1:O:267:GLY:HA3	2.43	0.53
1:P:149:LYS:HB2	1:P:281:GLY:O	2.08	0.53
1:G:37:HIS:O	1:O:185:TYR:HE2	1.92	0.53
1:N:252:GLN:HG3	6:N:2954:HOH:O	2.09	0.53
1:Q:39:ASN:HB2	1:Q:83:LYS:O	2.09	0.53
1:A:267:GLY:O	1:A:271:VAL:HG23	2.09	0.53
1:Q:109:HIS:O	1:Q:110:HIS:HB2	2.09	0.53
1:H:253:LYS:HE3	6:H:1024:HOH:O	2.09	0.53
1:L:316:HIS:CG	1:L:317:PRO:HD2	2.44	0.53
1:N:40:VAL:HG12	1:N:104:CYS:SG	2.48	0.53
1:A:69:GLN:NE2	1:A:73:ASP:OD1	2.42	0.52
1:C:175:GLY:O	1:C:177:LYS:HE2	2.09	0.52
1:I:361:VAL:O	1:I:365:VAL:HG23	2.09	0.52
1:E:168:VAL:HG13	1:E:280:HIS:ND1	2.23	0.52
1:B:205:PHE:HD2	1:B:239:TRP:CD2	2.27	0.52
1:A:238:VAL:HG22	1:A:248:VAL:HG22	1.92	0.52
1:K:25:PHE:CD1	1:L:160:ALA:HB1	2.44	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:I:109:HIS:O	1:I:110:HIS:HB2	2.09	0.52
1:J:283:MET:HG2	1:J:291:ILE:HB	1.89	0.52
1:E:312:PHE:CZ	1:E:379:GLU:HG3	2.43	0.52
1:K:34:LEU:HA	1:K:37:HIS:ND1	2.23	0.52
1:P:206:GLU:HG3	1:P:207:LYS:O	2.10	0.52
1:P:182:GLY:HA3	1:P:229:TRP:CZ2	2.44	0.52
1:F:137:VAL:CG1	1:F:306:VAL:HB	2.39	0.52
1:D:313:LEU:HD22	1:D:319:PHE:CD1	2.44	0.52
1:H:105:ILE:HG12	1:H:298:MET:HE3	1.91	0.52
1:N:49:LEU:HD21	1:N:99:GLU:HG2	1.91	0.52
1:H:146:ARG:HD2	1:H:290:TYR:CD1	2.45	0.52
1:C:143:ARG:HG3	6:C:1049:HOH:O	2.09	0.52
1:I:303:ARG:NH2	3:I:609:ADP:O2A	2.41	0.52
1:L:205:PHE:CD1	1:L:242:GLU:HG3	2.44	0.52
1:F:176:LEU:HD12	1:F:229:TRP:CZ2	2.45	0.52
1:M:331:ARG:NH1	3:M:613:ADP:O2A	2.42	0.52
1:N:184:TYR:CE1	1:N:240:ILE:HD12	2.45	0.52
1:G:35:SER:HB3	1:O:186:PRO:HG2	1.90	0.52
1:H:285:ASN:HB2	1:H:291:ILE:HD11	1.92	0.52
1:C:84:THR:HG22	1:C:86:CYS:SG	2.49	0.52
1:C:309:ARG:NH1	1:C:342:ASP:O	2.42	0.52
1:N:143:ARG:HG3	6:N:1155:HOH:O	2.09	0.52
1:K:132:PHE:CZ	1:K:365:VAL:HG22	2.45	0.52
1:E:50:TYR:O	1:E:54:TRP:HB3	2.10	0.52
1:I:121:ASP:HB3	1:I:356:SER:HB2	1.92	0.52
1:C:27:ALA:HB2	1:C:54:TRP:NE1	2.25	0.52
1:F:247:ARG:NH1	3:F:606:ADP:O1B	2.43	0.52
1:Q:356:SER:O	1:Q:360:LEU:HG	2.10	0.52
1:F:188:THR:HG22	1:F:223:PRO:HG2	1.92	0.52
1:B:183:LYS:HG2	1:B:184:TYR:H	1.73	0.52
1:R:145:GLY:O	1:R:146:ARG:HD3	2.09	0.52
1:K:31:PHE:CE2	1:K:47:LYS:HG2	2.44	0.52
1:N:342:ASP:O	1:N:343:SER:HB2	2.09	0.52
1:E:109:HIS:HE1	1:E:296:THR:O	1.93	0.52
1:G:161:GLU:O	1:G:165:VAL:HG23	2.09	0.52
1:C:188:THR:HG22	1:C:223:PRO:HG2	1.91	0.52
1:F:220:ARG:O	1:F:222:TRP:N	2.43	0.52
1:E:113:PRO:HA	1:E:287:ARG:HH22	1.75	0.52
1:E:105:ILE:HG12	1:E:298:MET:HE2	1.92	0.52
1:F:173:LEU:HD13	1:F:229:TRP:CG	2.44	0.52
1:D:229:TRP:HB3	1:D:238:VAL:HB	1.91	0.52
1:B:384:ILE:HA	1:B:387:MET:HG3	1.92	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:L:184:TYR:CD2	1:L:186:PRO:HD3	2.45	0.51
1:I:143:ARG:HA	1:I:248:VAL:O	2.11	0.51
1:I:238:VAL:HA	1:I:247:ARG:O	2.10	0.51
1:N:364:LEU:HD22	1:N:368:VAL:CG2	2.39	0.51
1:L:143:ARG:NH2	1:L:297:ASN:OD1	2.43	0.51
1:E:24:LYS:HE3	1:E:25:PHE:CE2	2.44	0.51
1:H:202:HIS:HB3	3:H:608:ADP:H1'	1.91	0.51
1:B:26:LYS:O	1:B:29:ASP:HB2	2.10	0.51
1:L:111:PHE:CE1	1:L:115:ASP:HB3	2.45	0.51
1:D:8:TYR:HD2	1:D:11:LYS:NZ	2.08	0.51
1:D:34:LEU:HA	1:D:37:HIS:ND1	2.26	0.51
1:A:313:LEU:O	1:A:313:LEU:HD23	2.10	0.51
1:C:177:LYS:HD2	1:H:43:SER:CB	2.41	0.51
1:E:357:GLU:O	1:E:361:VAL:HG23	2.11	0.51
1:N:10:VAL:HG12	1:N:11:LYS:N	2.25	0.51
1:B:236:PHE:CZ	1:B:267:GLY:HA3	2.45	0.51
1:B:99:GLU:O	1:B:99:GLU:HG2	2.09	0.51
1:E:66:LYS:O	1:E:66:LYS:HD3	2.10	0.51
1:L:144:CYS:HA	1:L:301:VAL:O	2.09	0.51
1:P:361:VAL:O	1:P:365:VAL:HG23	2.11	0.51
1:M:318:ARG:HD3	1:M:388:ILE:HD13	1.92	0.51
1:O:278:CYS:CB	1:O:280:HIS:CE1	2.93	0.51
1:E:377:LYS:HG2	6:E:2760:HOH:O	2.11	0.51
1:F:112:LYS:O	1:F:115:ASP:HB2	2.11	0.51
1:E:184:TYR:CE1	1:E:240:ILE:HD12	2.46	0.51
1:P:18:LYS:HB3	1:P:20:TRP:CE2	2.46	0.51
1:E:91:GLU:HB2	1:E:283:MET:CE	2.41	0.51
1:H:31:PHE:CD1	1:H:32:PRO:HD2	2.46	0.51
1:O:285:ASN:HB3	1:O:288:LEU:HB2	1.93	0.51
1:L:180:LEU:O	1:L:229:TRP:HH2	1.92	0.51
1:F:44:GLN:OE1	1:F:44:GLN:HA	2.11	0.51
1:C:48:GLU:HB2	6:C:3133:HOH:O	2.09	0.51
1:K:204:LEU:HD12	1:K:205:PHE:H	1.76	0.51
1:L:282:LEU:O	1:L:283:MET:C	2.49	0.51
1:G:310:LEU:O	1:G:314:GLU:HB3	2.11	0.51
1:N:306:VAL:HG23	1:N:308:LEU:HB2	1.93	0.51
1:O:140:CYS:SG	1:O:306:VAL:HG12	2.51	0.51
1:F:297:ASN:HB3	1:F:301:VAL:HG13	1.93	0.50
1:C:166:GLU:OE1	1:C:225:GLY:HA2	2.10	0.50
1:M:60:ASN:ND2	1:M:90:ASP:OD2	2.41	0.50
1:P:351:ALA:O	1:P:360:LEU:HD22	2.11	0.50
1:B:20:TRP:CG	1:B:55:ASP:HB3	2.45	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:284:HIS:HE1	6:B:3038:HOH:O	1.93	0.50
1:C:313:LEU:HD11	1:C:322:MET:HE1	1.92	0.50
1:I:183:LYS:HG2	1:I:184:TYR:N	2.25	0.50
1:H:141:ARG:HD3	3:H:608:ADP:C8	2.46	0.50
1:A:91:GLU:OE2	1:A:149:LYS:HE2	2.11	0.50
1:H:140:CYS:HB3	1:H:257:LEU:HD23	1.93	0.50
1:J:166:GLU:CD	1:J:225:GLY:HA2	2.32	0.50
1:D:320:ASP:OD1	1:D:330:LYS:NZ	2.40	0.50
1:O:244:ASP:OD1	1:O:292:CYS:HB3	2.11	0.50
1:I:257:LEU:HD11	1:I:364:LEU:HD12	1.93	0.50
1:G:318:ARG:HD3	1:G:388:ILE:HD13	1.94	0.50
1:R:308:LEU:CD1	1:R:310:LEU:HD11	2.40	0.50
1:Q:154:PRO:HG2	1:Q:243:GLU:O	2.12	0.50
1:F:39:ASN:HB2	1:F:83:LYS:O	2.11	0.50
1:K:127:LEU:HD23	1:K:258:LYS:HG3	1.92	0.50
1:D:154:PRO:HD2	1:D:293:THR:OG1	2.12	0.50
1:A:346:ASP:OD1	1:A:346:ASP:C	2.50	0.50
1:C:108:ILE:CG2	1:C:296:THR:HG22	2.40	0.50
1:D:143:ARG:NH2	1:D:297:ASN:OD1	2.45	0.50
1:J:245:HIS:C	1:J:246:ILE:HG13	2.32	0.50
1:A:151:VAL:HG12	1:A:152:CYS:O	2.12	0.50
1:C:177:LYS:HD2	1:H:43:SER:HA	1.94	0.50
1:D:229:TRP:O	1:D:238:VAL:N	2.43	0.50
1:R:364:LEU:HD22	1:R:368:VAL:HG23	1.93	0.50
1:K:346:ASP:C	1:K:346:ASP:OD1	2.49	0.50
1:Q:145:GLY:H	1:Q:301:VAL:HG12	1.76	0.50
1:Q:314:GLU:CG	1:Q:315:LYS:HD2	2.41	0.50
1:P:126:LYS:HD2	1:Q:366:ASP:OD2	2.11	0.50
1:P:45:LEU:HD11	1:P:50:TYR:HB2	1.93	0.50
1:B:316:HIS:CG	1:B:317:PRO:HD2	2.46	0.50
1:F:135:LYS:O	1:F:135:LYS:HG2	2.11	0.50
1:A:297:ASN:HB3	1:A:301:VAL:HG13	1.94	0.50
1:Q:79:PHE:HB3	6:Q:1291:HOH:O	2.11	0.50
1:P:232:ASN:HB2	6:P:1394:HOH:O	2.11	0.50
1:J:158:SER:OG	1:J:161:GLU:HG3	2.12	0.50
1:A:57:VAL:CG1	1:A:61:GLY:HA2	2.41	0.50
1:F:18:LYS:HD3	1:F:20:TRP:HZ2	1.74	0.50
1:G:357:GLU:CD	1:G:357:GLU:H	2.15	0.50
1:G:142:ILE:HG22	1:G:264:PHE:CE1	2.47	0.50
1:K:250:SER:CB	1:K:264:PHE:HB2	2.42	0.50
1:R:284:HIS:CD2	1:R:285:ASN:O	2.64	0.50
1:A:314:GLU:CG	1:A:315:LYS:HD2	2.41	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:355:LYS:HB2	1:E:360:LEU:HD21	1.93	0.50
1:I:62:VAL:HG11	1:I:89:GLY:HA3	1.93	0.50
1:B:364:LEU:HD22	1:B:368:VAL:HG23	1.94	0.50
1:A:47:LYS:O	1:A:51:GLU:HB2	2.12	0.50
1:C:121:ASP:OD2	1:C:358:ARG:HD3	2.12	0.50
1:P:141:ARG:HG3	1:P:251:MET:HB3	1.93	0.50
1:N:69:GLN:NE2	1:N:73:ASP:OD1	2.43	0.50
1:B:297:ASN:HB3	1:B:301:VAL:HG13	1.93	0.50
1:R:183:LYS:HD3	1:R:185:TYR:CE2	2.46	0.50
1:A:40:VAL:HB	1:A:84:THR:HA	1.94	0.50
1:A:66:LYS:HE3	1:B:16:HIS:CD2	2.47	0.50
1:R:277:GLU:HG2	1:R:277:GLU:O	2.11	0.50
1:F:18:LYS:HB3	1:F:20:TRP:CZ2	2.47	0.49
1:E:288:LEU:CD2	1:E:353:LEU:HD11	2.42	0.49
1:F:303:ARG:NH2	3:F:606:ADP:O2A	2.45	0.49
1:M:313:LEU:HD21	1:M:319:PHE:CD1	2.47	0.49
1:E:240:ILE:HA	1:E:245:HIS:O	2.12	0.49
1:M:228:ILE:HD11	1:M:237:LEU:HD23	1.93	0.49
1:N:143:ARG:NH2	1:N:297:ASN:OD1	2.45	0.49
1:A:247:ARG:NH1	3:A:601:ADP:O1B	2.43	0.49
1:E:177:LYS:HD3	6:E:2542:HOH:O	2.11	0.49
1:C:224:ASP:O	1:C:226:ARG:HD2	2.12	0.49
1:B:152:CYS:HB2	1:B:161:GLU:OE1	2.13	0.49
1:R:105:ILE:CD1	1:R:298:MET:HE1	2.42	0.49
1:J:49:LEU:HD21	1:J:99:GLU:HG2	1.94	0.49
1:P:278:CYS:HB3	1:P:280:HIS:CE1	2.48	0.49
1:J:285:ASN:ND2	1:J:287:ARG:H	2.10	0.49
1:B:239:TRP:HH2	3:B:602:ADP:H5'2	1.76	0.49
1:G:184:TYR:CE1	1:G:240:ILE:HD12	2.47	0.49
1:M:313:LEU:C	1:M:313:LEU:HD23	2.32	0.49
1:B:357:GLU:O	1:B:361:VAL:HG23	2.13	0.49
1:B:377:LYS:HG3	1:B:387:MET:CE	2.42	0.49
1:E:188:THR:HG22	1:E:223:PRO:HG2	1.93	0.49
1:A:98:LYS:HE3	1:A:102:ASP:OD2	2.12	0.49
1:P:267:GLY:O	1:P:271:VAL:HG23	2.12	0.49
1:I:285:ASN:ND2	1:I:288:LEU:H	2.03	0.49
1:G:126:LYS:HB2	1:G:358:ARG:HD2	1.94	0.49
1:K:257:LEU:HD11	1:K:364:LEU:HD12	1.95	0.49
1:R:143:ARG:HG3	6:R:1003:HOH:O	2.11	0.49
1:C:151:VAL:CG1	1:C:152:CYS:N	2.75	0.49
1:G:38:ASN:C	1:G:38:ASN:HD22	2.16	0.49
1:H:372:ILE:CG2	1:H:376:LYS:HE2	2.43	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:K:94:TYR:CD1	1:K:95:GLU:HG2	2.47	0.49
1:J:318:ARG:HD3	1:J:388:ILE:CD1	2.41	0.49
1:H:322:MET:O	1:H:326:LEU:HG	2.13	0.49
1:B:331:ARG:NH1	1:B:336:GLU:HB2	2.28	0.49
1:M:67:CYS:HB3	1:M:87:VAL:O	2.12	0.49
1:K:154:PRO:N	1:K:155:PRO:HD2	2.27	0.49
1:E:113:PRO:HA	1:E:287:ARG:NH2	2.28	0.49
1:E:24:LYS:HE3	1:E:25:PHE:HE2	1.77	0.49
1:D:121:ASP:HB3	1:D:356:SER:HB2	1.94	0.49
1:R:147:SER:HB2	1:R:283:MET:HB2	1.95	0.49
1:F:177:LYS:HA	1:F:181:ALA:HB2	1.95	0.49
1:L:142:ILE:HG22	1:L:142:ILE:O	2.12	0.49
1:E:247:ARG:NH1	3:E:605:ADP:O1B	2.46	0.49
1:Q:303:ARG:NH2	3:Q:617:ADP:O2A	2.45	0.49
1:M:143:ARG:HG3	6:M:1485:HOH:O	2.13	0.49
1:F:139:SER:HA	1:F:254:GLY:O	2.12	0.49
1:O:297:ASN:HB3	1:O:301:VAL:HG13	1.94	0.49
1:B:321:GLU:O	1:B:325:LYS:HG3	2.13	0.49
1:D:141:ARG:HG3	1:D:251:MET:HB3	1.95	0.49
1:J:346:ASP:OD1	1:J:346:ASP:C	2.51	0.49
1:P:285:ASN:ND2	1:P:288:LEU:H	2.09	0.49
1:L:187:LEU:HB3	1:L:226:ARG:O	2.12	0.49
1:M:212:LEU:HB3	6:M:2758:HOH:O	2.11	0.49
1:F:316:HIS:CD2	1:F:384:ILE:HD11	2.48	0.49
1:M:146:ARG:HA	6:M:2237:HOH:O	2.12	0.49
1:E:308:LEU:HD13	1:E:310:LEU:HD21	1.94	0.49
1:I:287:ARG:NH1	6:I:2239:HOH:O	2.44	0.49
1:E:141:ARG:HG3	1:E:251:MET:HB3	1.95	0.49
1:D:322:MET:HG3	1:D:389:PRO:CD	2.41	0.49
1:O:49:LEU:HD21	1:O:99:GLU:HG2	1.95	0.49
1:G:314:GLU:HG3	1:G:315:LYS:HD2	1.94	0.49
1:K:346:ASP:HB2	6:K:1019:HOH:O	2.11	0.49
1:I:52:LYS:HE2	1:I:53:TYR:CE2	2.48	0.49
1:H:309:ARG:HG2	6:H:2419:HOH:O	2.12	0.49
1:L:303:ARG:HA	1:L:349:ASN:HD21	1.78	0.49
1:M:250:SER:HB3	1:M:264:PHE:HB2	1.94	0.49
1:M:69:GLN:HG3	1:M:69:GLN:O	2.11	0.49
1:M:38:ASN:HD21	1:M:82:LYS:HE3	1.78	0.49
1:A:89:GLY:HA2	1:A:155:PRO:HG2	1.95	0.49
1:A:156:ALA:HB1	1:B:16:HIS:HA	1.95	0.49
1:O:81:GLY:HA2	6:O:1408:HOH:O	2.11	0.49
1:J:312:PHE:CZ	1:J:379:GLU:HG3	2.48	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:R:66:LYS:HD3	1:R:66:LYS:O	2.12	0.49
1:I:36:LYS:HG2	1:Q:189:THR:HB	1.95	0.48
1:E:331:ARG:NH1	3:E:605:ADP:O2A	2.45	0.48
1:Q:26:LYS:O	1:Q:29:ASP:HB2	2.13	0.48
1:D:171:ASP:O	1:D:174:GLY:N	2.46	0.48
1:C:168:VAL:HG13	1:C:280:HIS:CE1	2.48	0.48
1:M:34:LEU:HD13	1:M:42:ALA:CB	2.42	0.48
1:I:94:TYR:CZ	1:I:288:LEU:HD11	2.48	0.48
1:I:297:ASN:HB3	1:I:301:VAL:CG1	2.43	0.48
1:E:151:VAL:HG13	1:E:152:CYS:H	1.78	0.48
1:A:153:LEU:HB3	1:A:155:PRO:HD2	1.95	0.48
1:M:307:HIS:CE1	3:M:613:ADP:C2	3.01	0.48
1:I:242:GLU:HB3	6:I:1538:HOH:O	2.13	0.48
1:B:284:HIS:CD2	1:B:285:ASN:O	2.66	0.48
1:N:139:SER:OG	3:N:614:ADP:N1	2.45	0.48
1:A:236:PHE:CE1	1:A:267:GLY:HA3	2.48	0.48
1:K:168:VAL:HG13	1:K:280:HIS:CE1	2.48	0.48
1:O:354:GLY:O	1:O:355:LYS:HG3	2.13	0.48
1:H:110:HIS:HE1	6:H:1515:HOH:O	1.96	0.48
1:B:94:TYR:OH	1:B:287:ARG:NH1	2.42	0.48
1:A:288:LEU:O	1:A:299:GLY:HA2	2.13	0.48
1:I:374:CYS:HB3	1:I:384:ILE:HD13	1.95	0.48
1:G:247:ARG:NH1	3:G:607:ADP:O1B	2.46	0.48
1:C:318:ARG:HD3	1:C:388:ILE:HD13	1.95	0.48
1:F:301:VAL:O	1:F:301:VAL:HG12	2.13	0.48
1:K:105:ILE:CD1	1:K:298:MET:HE1	2.43	0.48
1:K:153:LEU:C	1:K:155:PRO:HD2	2.34	0.48
1:F:384:ILE:HA	1:F:387:MET:HG3	1.94	0.48
1:M:226:ARG:HG3	1:M:241:ASN:O	2.13	0.48
1:B:327:ARG:NH1	1:B:350:TRP:CD1	2.81	0.48
1:H:377:LYS:HG3	1:H:387:MET:HE2	1.96	0.48
1:C:151:VAL:HG12	1:C:152:CYS:N	2.29	0.48
1:L:250:SER:HB3	1:L:264:PHE:HB2	1.96	0.48
1:M:213:LEU:HD12	1:M:218:CYS:HB2	1.94	0.48
1:L:293:THR:HB	6:L:1525:HOH:O	2.13	0.48
1:A:285:ASN:HB3	1:A:288:LEU:HB2	1.95	0.48
1:M:191:ASN:HD21	1:M:193:LYS:H	1.59	0.48
1:Q:151:VAL:HG12	1:Q:245:HIS:CE1	2.48	0.48
1:D:33:ASP:O	1:D:34:LEU:HD23	2.14	0.48
1:C:201:ASP:O	1:C:202:HIS:HB2	2.12	0.48
1:C:111:PHE:CG	1:C:353:LEU:HD13	2.48	0.48
1:B:322:MET:HE2	1:B:388:ILE:HG12	1.94	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:312:PHE:CZ	1:C:379:GLU:HG3	2.49	0.48
1:Q:101:PHE:O	1:Q:105:ILE:HG13	2.13	0.48
1:J:91:GLU:OE2	1:J:149:LYS:HG3	2.13	0.48
1:L:213:LEU:HD13	6:L:1412:HOH:O	2.13	0.48
1:I:328:LEU:HD11	1:I:367:GLY:HA3	1.96	0.48
1:E:154:PRO:HG2	1:E:243:GLU:O	2.13	0.48
1:B:39:ASN:O	1:B:40:VAL:C	2.51	0.48
1:A:143:ARG:NH2	1:A:297:ASN:OD1	2.47	0.48
1:O:109:HIS:O	1:O:110:HIS:HB2	2.14	0.48
1:I:313:LEU:HD12	1:I:371:LEU:O	2.13	0.48
1:I:331:ARG:HB2	1:I:346:ASP:HB3	1.95	0.48
1:K:49:LEU:HD21	1:K:99:GLU:CG	2.40	0.48
1:M:32:PRO:HD3	1:N:159:ARG:HH21	1.78	0.48
1:B:377:LYS:HG3	1:B:387:MET:HE2	1.96	0.48
1:I:180:LEU:O	1:I:229:TRP:HH2	1.97	0.48
1:C:237:LEU:N	1:C:237:LEU:HD12	2.29	0.48
1:A:146:ARG:NH2	1:A:268:LEU:HD21	2.29	0.48
1:F:113:PRO:HA	1:F:287:ARG:NH2	2.28	0.48
1:M:270:GLU:OE1	1:M:273:ARG:NH1	2.47	0.48
1:J:18:LYS:O	1:J:21:GLU:HG2	2.14	0.48
1:C:154:PRO:HG2	1:C:243:GLU:O	2.14	0.48
1:E:88:PHE:HD1	1:E:292:CYS:O	1.97	0.48
1:I:113:PRO:HA	1:I:287:ARG:NH2	2.28	0.48
1:Q:154:PRO:HD3	1:Q:245:HIS:CD2	2.49	0.48
1:L:165:VAL:HB	1:L:241:ASN:HD21	1.79	0.48
1:G:359:GLU:O	1:G:363:VAL:HG23	2.14	0.48
1:K:191:ASN:ND2	1:K:193:LYS:H	2.11	0.48
1:C:313:LEU:HD13	1:C:374:CYS:HB3	1.96	0.48
1:R:384:ILE:CA	1:R:387:MET:HG3	2.44	0.48
1:K:143:ARG:HG2	1:K:144:CYS:N	2.28	0.48
1:K:143:ARG:HG3	6:K:1071:HOH:O	2.14	0.48
1:I:205:PHE:CD1	1:I:242:GLU:HG3	2.49	0.48
1:M:66:LYS:O	1:M:66:LYS:HD3	2.14	0.48
1:P:285:ASN:ND2	1:P:288:LEU:HG	2.29	0.47
1:K:285:ASN:HD21	1:K:287:ARG:HB2	1.79	0.47
1:E:94:TYR:CZ	1:E:288:LEU:HD11	2.48	0.47
1:K:184:TYR:CD2	1:K:186:PRO:HD3	2.49	0.47
1:G:211:ALA:O	1:G:215:THR:HG23	2.14	0.47
1:A:183:LYS:HD3	1:A:185:TYR:CE2	2.49	0.47
1:J:176:LEU:C	1:J:177:LYS:HG2	2.34	0.47
1:J:94:TYR:OH	1:J:287:ARG:NH1	2.46	0.47
1:F:305:SER:HB3	1:F:348:SER:CB	2.35	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:143:ARG:NH1	3:G:607:ADP:O3B	2.48	0.47
1:P:18:LYS:HD2	1:P:21:GLU:OE2	2.14	0.47
1:E:208:PRO:HG3	1:E:222:TRP:CE2	2.49	0.47
1:F:314:GLU:OE2	1:F:343:SER:HB3	2.14	0.47
1:Q:195:GLN:NE2	6:Q:1708:HOH:O	2.47	0.47
1:G:236:PHE:CZ	1:G:267:GLY:HA3	2.49	0.47
1:J:153:LEU:HD22	6:J:2386:HOH:O	2.13	0.47
1:E:288:LEU:HD22	1:E:353:LEU:HD11	1.96	0.47
1:C:98:LYS:HE3	1:C:102:ASP:OD2	2.14	0.47
1:I:364:LEU:HD22	1:I:364:LEU:O	2.14	0.47
1:M:34:LEU:HD13	1:M:42:ALA:HB2	1.96	0.47
1:I:105:ILE:HD13	1:I:298:MET:HE1	1.95	0.47
1:D:187:LEU:HB3	1:D:223:PRO:HB2	1.95	0.47
1:L:126:LYS:HB2	1:L:358:ARG:HD3	1.95	0.47
1:K:312:PHE:CZ	1:K:379:GLU:HG3	2.49	0.47
1:Q:295:PRO:O	1:Q:298:MET:HE2	2.14	0.47
1:K:52:LYS:HE2	1:K:53:TYR:CE2	2.49	0.47
1:O:34:LEU:HD12	6:O:2791:HOH:O	2.13	0.47
1:K:204:LEU:HD13	1:K:228:ILE:HB	1.97	0.47
1:F:226:ARG:HG3	1:F:241:ASN:O	2.14	0.47
1:R:38:ASN:HA	6:R:2601:HOH:O	2.14	0.47
1:N:331:ARG:HB2	1:N:346:ASP:HB3	1.96	0.47
1:G:213:LEU:CD1	1:G:218:CYS:HB2	2.38	0.47
1:M:285:ASN:HD22	1:M:285:ASN:C	2.18	0.47
1:L:195:GLN:O	1:L:199:ILE:HG13	2.15	0.47
1:B:137:VAL:CG1	1:B:255:GLY:HA2	2.45	0.47
1:I:50:TYR:O	1:I:54:TRP:HB3	2.14	0.47
1:G:257:LEU:O	1:G:257:LEU:HD22	2.14	0.47
1:Q:285:ASN:ND2	1:Q:288:LEU:HG	2.30	0.47
1:L:378:LEU:HD21	1:L:384:ILE:HG23	1.96	0.47
1:P:285:ASN:HD22	1:P:288:LEU:CB	2.28	0.47
1:L:147:SER:HB2	1:L:283:MET:HB2	1.96	0.47
1:F:230:HIS:CB	1:F:237:LEU:HD23	2.45	0.47
1:A:143:ARG:O	1:A:302:VAL:HA	2.15	0.47
1:N:70:THR:HG21	1:N:212:LEU:HD13	1.96	0.47
1:P:318:ARG:NH1	1:P:385:ASP:OD2	2.48	0.47
1:M:101:PHE:O	1:M:105:ILE:HG13	2.15	0.47
1:D:94:TYR:CZ	1:D:288:LEU:HD11	2.50	0.47
1:K:188:THR:CG2	1:K:223:PRO:HG2	2.42	0.47
1:K:285:ASN:ND2	1:K:288:LEU:H	2.12	0.47
1:F:250:SER:CB	1:F:264:PHE:HB2	2.43	0.47
1:A:303:ARG:NE	3:A:601:ADP:O3B	2.46	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:I:239:TRP:HB2	1:I:247:ARG:HB2	1.96	0.47
1:H:186:PRO:HG2	1:P:35:SER:HB3	1.97	0.47
1:B:55:ASP:N	1:B:55:ASP:OD1	2.47	0.47
1:I:27:ALA:HB2	1:I:54:TRP:NE1	2.29	0.47
1:H:242:GLU:CG	1:H:243:GLU:H	2.26	0.47
1:P:210:GLY:O	1:P:214:THR:HG23	2.15	0.47
1:R:184:TYR:CE1	1:R:240:ILE:HD12	2.50	0.47
1:M:74:ASN:OD1	1:M:211:ALA:HB1	2.14	0.47
1:K:157:MET:HE3	1:K:245:HIS:HE2	1.80	0.47
1:O:136:TYR:O	1:O:308:LEU:HD23	2.15	0.47
1:L:370:LEU:O	1:L:373:ALA:HB3	2.15	0.47
1:R:346:ASP:OD1	1:R:346:ASP:C	2.51	0.47
1:H:364:LEU:O	1:H:368:VAL:HG23	2.15	0.47
1:F:182:GLY:HA3	1:F:230:HIS:O	2.15	0.47
1:I:83:LYS:HD3	1:I:83:LYS:HA	1.38	0.47
3:K:611:ADP:O1B	5:K:811:NO3:O2	2.33	0.47
1:D:77:ASN:ND2	1:D:83:LYS:HE2	2.30	0.47
1:D:312:PHE:CZ	1:D:379:GLU:HG3	2.49	0.47
1:Q:202:HIS:HB3	3:Q:617:ADP:H1'	1.95	0.47
1:N:361:VAL:O	1:N:365:VAL:HG23	2.15	0.47
1:C:228:ILE:HD11	1:C:237:LEU:HD23	1.95	0.47
1:B:111:PHE:CD2	1:B:353:LEU:HD13	2.50	0.47
1:O:88:PHE:CE2	1:O:94:TYR:HB2	2.50	0.47
1:C:326:LEU:O	1:C:327:ARG:HB2	2.14	0.47
1:L:298:MET:CE	1:L:353:LEU:HD12	2.38	0.47
1:E:116:LYS:HG3	1:E:287:ARG:HA	1.97	0.47
1:M:88:PHE:HD1	1:M:292:CYS:O	1.98	0.47
1:F:59:PRO:HD2	1:F:92:TYR:CG	2.50	0.47
1:R:38:ASN:OD1	1:R:82:LYS:HE3	2.14	0.47
1:O:136:TYR:HB3	1:O:308:LEU:CD2	2.44	0.47
1:G:162:ARG:HH12	1:G:221:ASP:HB2	1.80	0.47
1:L:20:TRP:CG	1:L:55:ASP:HB3	2.50	0.47
1:A:168:VAL:HG13	1:A:280:HIS:ND1	2.30	0.47
1:M:44:GLN:NE2	1:M:107:GLU:OE1	2.48	0.47
1:J:144:CYS:HA	1:J:301:VAL:O	2.14	0.46
1:C:244:ASP:OD1	1:C:292:CYS:HB3	2.15	0.46
1:E:205:PHE:CD1	1:E:242:GLU:HG3	2.50	0.46
1:E:142:ILE:HD12	1:E:261:PHE:HA	1.97	0.46
1:D:368:VAL:O	1:D:372:ILE:HG13	2.16	0.46
1:G:141:ARG:NH2	6:G:1518:HOH:O	2.46	0.46
1:N:88:PHE:HD2	1:N:93:SER:HB3	1.80	0.46
1:M:364:LEU:HD22	1:M:368:VAL:HG23	1.97	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:184:TYR:OH	1:D:227:GLY:HA3	2.14	0.46
1:A:195:GLN:O	1:A:199:ILE:HG13	2.15	0.46
1:A:87:VAL:HB	1:A:293:THR:HG22	1.96	0.46
1:E:309:ARG:NH1	1:E:342:ASP:OD1	2.48	0.46
1:B:53:TYR:CE2	1:B:97:TYR:HA	2.50	0.46
1:M:133:GLU:HB2	6:M:1530:HOH:O	2.15	0.46
1:P:154:PRO:HG2	1:P:243:GLU:O	2.15	0.46
1:J:155:PRO:HB3	1:J:216:SER:O	2.15	0.46
1:Q:285:ASN:ND2	1:Q:287:ARG:H	2.14	0.46
1:Q:247:ARG:HG2	6:Q:1471:HOH:O	2.16	0.46
1:C:105:ILE:HG12	1:C:298:MET:HE1	1.98	0.46
1:A:66:LYS:NZ	1:A:216:SER:O	2.48	0.46
1:N:77:ASN:ND2	1:N:83:LYS:HE2	2.30	0.46
1:D:137:VAL:HG13	1:D:306:VAL:HB	1.98	0.46
1:A:372:ILE:HG22	1:A:376:LYS:HE2	1.97	0.46
1:N:297:ASN:O	1:N:301:VAL:HG22	2.16	0.46
1:M:229:TRP:HB3	1:M:238:VAL:HB	1.98	0.46
1:D:45:LEU:O	1:I:178:GLY:HA2	2.16	0.46
1:L:326:LEU:O	1:L:327:ARG:HB2	2.14	0.46
1:O:319:PHE:HB3	6:O:2548:HOH:O	2.14	0.46
1:F:267:GLY:O	1:F:271:VAL:HG23	2.14	0.46
1:N:54:TRP:CD1	1:N:55:ASP:N	2.83	0.46
1:C:331:ARG:HB2	1:C:346:ASP:HB3	1.97	0.46
1:H:28:ALA:HB2	6:H:2750:HOH:O	2.14	0.46
1:B:116:LYS:HG3	1:B:287:ARG:HA	1.98	0.46
1:H:285:ASN:ND2	1:H:288:LEU:H	2.02	0.46
1:Q:143:ARG:NH1	1:Q:303:ARG:HD3	2.30	0.46
1:E:312:PHE:CE2	1:E:379:GLU:HA	2.50	0.46
1:K:304:ALA:O	1:K:348:SER:HB2	2.15	0.46
1:E:143:ARG:HG3	6:E:3012:HOH:O	2.16	0.46
1:L:313:LEU:CD2	1:L:319:PHE:CD1	2.98	0.46
1:L:377:LYS:HG3	1:L:387:MET:CE	2.45	0.46
1:L:190:MET:SD	1:L:195:GLN:HB2	2.56	0.46
1:R:314:GLU:HG3	1:R:315:LYS:HD2	1.97	0.46
1:I:297:ASN:C	1:I:301:VAL:HG13	2.35	0.46
1:H:184:TYR:CE2	1:H:186:PRO:HD3	2.51	0.46
1:R:105:ILE:HG12	1:R:298:MET:CE	2.46	0.46
1:M:157:MET:CE	1:M:161:GLU:HB3	2.45	0.46
1:Q:27:ALA:HB2	1:Q:54:TRP:CD1	2.51	0.46
1:G:206:GLU:HG3	1:G:207:LYS:O	2.15	0.46
1:H:285:ASN:ND2	1:H:288:LEU:HG	2.30	0.46
1:G:285:ASN:ND2	1:G:287:ARG:N	2.50	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:I:40:VAL:O	1:I:44:GLN:HG2	2.16	0.46
1:O:152:CYS:O	1:O:157:MET:HE3	2.16	0.46
1:P:294:CYS:O	1:P:297:ASN:N	2.44	0.46
1:P:278:CYS:HB3	1:P:280:HIS:HE1	1.81	0.46
1:R:66:LYS:HE3	6:R:2561:HOH:O	2.15	0.46
1:N:124:HIS:O	1:N:258:LYS:HE3	2.15	0.46
1:A:326:LEU:O	1:A:327:ARG:HB2	2.14	0.46
1:P:312:PHE:CZ	1:P:379:GLU:HG3	2.51	0.46
1:C:148:VAL:HG21	1:C:165:VAL:HG13	1.97	0.46
1:D:222:TRP:HA	1:D:226:ARG:HH12	1.80	0.46
1:M:312:PHE:CZ	1:M:379:GLU:HG3	2.51	0.46
1:I:285:ASN:HD22	1:I:288:LEU:N	2.03	0.46
1:H:144:CYS:HA	1:H:301:VAL:O	2.16	0.46
1:Q:297:ASN:HB3	1:Q:301:VAL:HG13	1.97	0.46
1:I:191:ASN:ND2	1:I:193:LYS:HB2	2.30	0.46
1:I:110:HIS:CE1	1:I:327:ARG:NH1	2.84	0.46
1:B:267:GLY:O	1:B:271:VAL:HG23	2.15	0.46
1:J:80:TYR:HD1	1:J:331:ARG:HA	1.80	0.46
1:K:70:THR:HG21	1:K:212:LEU:CD1	2.46	0.46
1:I:340:ALA:HB2	1:I:345:TYR:CD2	2.50	0.46
1:B:31:PHE:CE1	1:B:47:LYS:HA	2.51	0.46
1:N:207:LYS:HB3	1:N:208:PRO:HD2	1.96	0.46
1:J:145:GLY:H	1:J:301:VAL:CG1	2.29	0.46
1:R:305:SER:HA	1:R:347:ILE:O	2.16	0.46
1:N:252:GLN:OE1	1:N:263:ARG:NH2	2.49	0.46
1:A:301:VAL:O	1:A:301:VAL:HG12	2.15	0.46
1:C:168:VAL:HG13	1:C:280:HIS:ND1	2.30	0.46
1:J:124:HIS:ND1	1:J:262:SER:HB2	2.31	0.46
1:O:151:VAL:HG12	1:O:245:HIS:CE1	2.50	0.46
1:I:226:ARG:HG3	1:I:241:ASN:O	2.16	0.46
1:H:361:VAL:O	1:H:365:VAL:HG23	2.16	0.46
1:D:242:GLU:CG	1:D:243:GLU:H	2.29	0.46
1:E:108:ILE:HG21	1:E:296:THR:HG22	1.98	0.46
1:N:298:MET:HB2	1:N:298:MET:HE2	1.76	0.46
1:B:144:CYS:HA	1:B:301:VAL:O	2.16	0.46
1:L:151:VAL:HG12	1:L:152:CYS:O	2.16	0.46
1:L:151:VAL:HG12	1:L:152:CYS:N	2.31	0.46
1:B:228:ILE:HG12	1:B:229:TRP:N	2.30	0.46
1:K:159:ARG:HB2	1:L:30:ASN:OD1	2.16	0.46
1:M:267:GLY:O	1:M:271:VAL:HG23	2.16	0.46
1:A:321:GLU:CG	1:A:325:LYS:HE3	2.46	0.45
1:G:240:ILE:O	1:G:241:ASN:HB2	2.15	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:K:313:LEU:HA	1:K:378:LEU:HD12	1.97	0.45
1:A:201:ASP:O	1:A:202:HIS:CB	2.64	0.45
1:P:13:ARG:NH1	1:P:156:ALA:O	2.44	0.45
1:B:60:ASN:HB2	1:B:90:ASP:OD2	2.16	0.45
1:O:70:THR:O	1:O:74:ASN:ND2	2.44	0.45
1:L:172:ALA:C	1:L:174:GLY:H	2.19	0.45
1:A:219:ALA:HB3	6:A:1059:HOH:O	2.15	0.45
1:F:352:ARG:HH11	1:F:352:ARG:CG	2.30	0.45
1:F:117:HIS:CE1	1:F:300:THR:HG23	2.51	0.45
1:L:158:SER:OG	1:L:161:GLU:HG3	2.16	0.45
1:E:186:PRO:HG2	1:E:189:THR:OG1	2.16	0.45
1:J:137:VAL:HG13	1:J:306:VAL:HB	1.98	0.45
1:P:83:LYS:HZ1	1:P:336:GLU:CG	2.29	0.45
1:Q:53:TYR:OH	1:Q:99:GLU:HB3	2.16	0.45
1:H:143:ARG:HG3	6:H:1174:HOH:O	2.16	0.45
1:K:313:LEU:CD2	1:K:319:PHE:CD1	3.00	0.45
1:E:208:PRO:HD3	1:E:222:TRP:CZ2	2.51	0.45
1:I:121:ASP:CB	1:I:356:SER:HB2	2.46	0.45
1:E:91:GLU:O	1:E:91:GLU:HG2	2.16	0.45
6:Q:2768:HOH:O	1:R:16:HIS:HB3	2.15	0.45
1:B:172:ALA:O	1:B:274:LEU:HD13	2.16	0.45
1:B:18:LYS:HB2	1:B:21:GLU:HG2	1.98	0.45
1:M:41:MET:HE2	1:M:71:GLY:HA3	1.97	0.45
1:L:105:ILE:O	1:L:109:HIS:HB2	2.16	0.45
1:L:301:VAL:HG12	1:L:301:VAL:O	2.16	0.45
1:N:297:ASN:ND2	6:N:1089:HOH:O	2.44	0.45
1:R:54:TRP:CD1	1:R:55:ASP:N	2.84	0.45
1:A:239:TRP:HB2	1:A:247:ARG:HB2	1.99	0.45
1:F:352:ARG:HH11	1:F:352:ARG:HG2	1.81	0.45
1:E:109:HIS:CE1	1:E:296:THR:O	2.69	0.45
1:M:385:ASP:HA	1:M:388:ILE:HD12	1.98	0.45
1:A:91:GLU:HB2	1:A:283:MET:SD	2.56	0.45
1:A:168:VAL:HG12	1:A:169:VAL:N	2.30	0.45
1:N:50:TYR:O	1:N:54:TRP:HB3	2.17	0.45
1:D:176:LEU:C	1:D:177:LYS:HG2	2.37	0.45
1:D:207:LYS:O	1:D:209:THR:N	2.43	0.45
1:P:145:GLY:H	1:P:301:VAL:CG1	2.30	0.45
1:R:47:LYS:O	1:R:51:GLU:HB2	2.16	0.45
1:Q:319:PHE:CZ	1:Q:323:LEU:HD11	2.52	0.45
1:O:264:PHE:CZ	1:O:268:LEU:HD22	2.51	0.45
1:R:309:ARG:HG2	6:R:2020:HOH:O	2.15	0.45
1:D:10:VAL:HG13	6:D:2572:HOH:O	2.16	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:J:183:LYS:HD3	1:J:185:TYR:CE2	2.52	0.45
1:F:44:GLN:NE2	1:F:107:GLU:OE1	2.50	0.45
1:D:364:LEU:O	1:D:368:VAL:HG23	2.16	0.45
1:N:98:LYS:HE3	1:N:102:ASP:OD2	2.16	0.45
1:N:143:ARG:HD3	1:N:303:ARG:HB3	1.99	0.45
1:G:151:VAL:HG12	1:G:152:CYS:O	2.17	0.45
1:G:313:LEU:CD2	1:G:319:PHE:CD1	2.99	0.45
1:M:270:GLU:OE2	1:M:273:ARG:HD3	2.16	0.45
1:F:314:GLU:HG3	1:F:315:LYS:HD2	1.97	0.45
1:D:222:TRP:HA	1:D:226:ARG:NH1	2.32	0.45
1:C:184:TYR:CE1	1:C:240:ILE:HD12	2.52	0.45
1:D:240:ILE:O	1:D:241:ASN:HB2	2.16	0.45
1:D:159:ARG:O	1:D:163:ARG:HG3	2.16	0.45
1:G:55:ASP:OD1	1:G:55:ASP:N	2.45	0.45
1:M:191:ASN:OD1	1:M:194:ASP:HB2	2.16	0.45
1:L:374:CYS:HB3	1:L:384:ILE:HG21	1.99	0.45
1:O:278:CYS:HB3	1:O:280:HIS:HE1	1.75	0.45
1:F:153:LEU:C	1:F:155:PRO:CD	2.85	0.45
1:P:191:ASN:ND2	6:P:2801:HOH:O	2.46	0.45
1:K:58:THR:C	1:K:60:ASN:H	2.20	0.45
1:G:175:GLY:O	1:G:177:LYS:HE2	2.17	0.45
1:H:157:MET:HA	1:H:161:GLU:OE1	2.16	0.45
1:B:176:LEU:HD21	1:B:270:GLU:HB3	1.99	0.45
6:Q:3098:HOH:O	1:R:188:THR:HG21	2.16	0.45
1:E:111:PHE:CD1	1:E:353:LEU:HD22	2.51	0.45
1:L:18:LYS:HA	1:L:19:PRO:HD2	1.79	0.45
1:R:184:TYR:OH	1:R:227:GLY:HA3	2.16	0.45
1:D:300:THR:HB	1:D:302:VAL:HG23	1.97	0.45
1:Q:308:LEU:O	1:Q:344:THR:HA	2.17	0.45
1:J:258:LYS:HB3	6:J:2970:HOH:O	2.16	0.45
1:F:319:PHE:CE1	1:F:323:LEU:HD11	2.51	0.45
1:I:33:ASP:OD1	1:I:33:ASP:C	2.56	0.45
1:L:377:LYS:HG3	1:L:387:MET:HE2	1.99	0.45
1:I:201:ASP:HB3	1:I:203:PHE:CD2	2.51	0.45
1:A:352:ARG:CG	1:A:352:ARG:HH11	2.29	0.45
1:I:151:VAL:HG13	1:I:161:GLU:HB3	1.98	0.45
1:A:66:LYS:HE3	1:B:16:HIS:NE2	2.32	0.45
1:G:267:GLY:O	1:G:271:VAL:HG23	2.16	0.45
1:J:377:LYS:HE3	1:J:382:GLN:HB3	1.98	0.45
1:E:268:LEU:O	1:E:272:GLU:HG3	2.17	0.45
1:R:271:VAL:O	1:R:275:MET:HG2	2.17	0.45
1:I:35:SER:HB3	1:Q:186:PRO:CG	2.47	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:141:ARG:HD3	3:E:605:ADP:C8	2.52	0.45
1:Q:143:ARG:NH2	1:Q:297:ASN:OD1	2.47	0.45
1:C:313:LEU:HA	1:C:378:LEU:HD12	1.99	0.45
1:B:143:ARG:O	1:B:302:VAL:HA	2.17	0.45
1:F:84:THR:OG1	1:F:296:THR:HG23	2.18	0.45
1:L:229:TRP:O	1:L:229:TRP:CE3	2.69	0.45
1:B:137:VAL:HG12	1:B:255:GLY:HA2	1.99	0.45
1:G:224:ASP:O	1:G:226:ARG:HD2	2.16	0.45
1:K:201:ASP:O	1:K:202:HIS:HB2	2.16	0.45
1:D:352:ARG:HH11	1:D:352:ARG:HG2	1.82	0.45
1:J:41:MET:SD	1:J:41:MET:C	2.95	0.45
1:L:141:ARG:NH1	3:L:612:ADP:O2B	2.49	0.44
1:A:57:VAL:HG12	1:A:58:THR:O	2.17	0.44
1:K:70:THR:O	1:K:74:ASN:ND2	2.42	0.44
1:P:71:GLY:HA3	1:P:85:GLY:O	2.17	0.44
1:G:312:PHE:HB2	1:G:375:ASP:OD1	2.17	0.44
1:E:132:PHE:HE2	1:E:369:ASN:OD1	2.00	0.44
1:G:201:ASP:HB3	1:G:203:PHE:CE2	2.52	0.44
1:D:213:LEU:HD12	1:D:218:CYS:HB3	1.98	0.44
1:K:205:PHE:CE2	1:K:239:TRP:HB3	2.51	0.44
1:K:152:CYS:O	1:K:157:MET:HE3	2.17	0.44
1:F:242:GLU:CD	1:F:243:GLU:H	2.18	0.44
1:D:326:LEU:HD11	1:D:370:LEU:HD23	1.98	0.44
1:F:349:ASN:HB2	6:F:1226:HOH:O	2.17	0.44
1:E:284:HIS:CD2	1:E:285:ASN:O	2.70	0.44
1:F:168:VAL:HG13	1:F:280:HIS:CE1	2.53	0.44
1:E:127:LEU:HB3	1:E:258:LYS:HE3	1.98	0.44
1:Q:152:CYS:SG	1:R:17:SER:HB3	2.57	0.44
1:A:126:LYS:H	1:A:126:LYS:HG2	1.62	0.44
1:R:226:ARG:HG3	1:R:241:ASN:O	2.17	0.44
1:Q:186:PRO:HG2	1:Q:189:THR:OG1	2.16	0.44
1:L:166:GLU:O	1:L:166:GLU:HG2	2.18	0.44
1:E:346:ASP:OD1	1:E:346:ASP:O	2.36	0.44
1:O:126:LYS:HB2	1:O:358:ARG:HD2	1.98	0.44
1:E:229:TRP:O	1:E:230:HIS:HB3	2.18	0.44
1:I:57:VAL:HG12	1:I:58:THR:N	2.33	0.44
1:F:31:PHE:HA	1:F:32:PRO:HD3	1.67	0.44
1:H:110:HIS:CE1	6:H:1515:HOH:O	2.69	0.44
1:G:210:GLY:HA2	6:G:1688:HOH:O	2.17	0.44
1:M:151:VAL:CG1	1:M:152:CYS:N	2.80	0.44
1:Q:318:ARG:HD3	1:Q:388:ILE:HD13	1.99	0.44
1:H:173:LEU:HD13	1:H:229:TRP:CG	2.52	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:79:PHE:CD2	1:D:337:SER:HA	2.52	0.44
1:I:94:TYR:CD1	1:I:95:GLU:HG2	2.53	0.44
1:F:18:LYS:HB3	1:F:20:TRP:CE2	2.52	0.44
1:G:313:LEU:HD12	1:G:374:CYS:HB2	1.98	0.44
1:N:105:ILE:HG12	1:N:298:MET:CE	2.46	0.44
1:I:110:HIS:HE1	6:I:3246:HOH:O	2.00	0.44
1:C:117:HIS:HB2	1:C:287:ARG:O	2.17	0.44
1:M:364:LEU:HD22	1:M:368:VAL:CG2	2.47	0.44
1:Q:268:LEU:O	1:Q:272:GLU:HG3	2.18	0.44
1:N:162:ARG:HG2	1:N:241:ASN:ND2	2.32	0.44
1:I:34:LEU:HA	1:I:37:HIS:ND1	2.33	0.44
1:L:135:LYS:HD3	1:L:136:TYR:CE1	2.52	0.44
1:O:313:LEU:O	1:O:313:LEU:HD22	2.17	0.44
1:J:285:ASN:ND2	1:J:288:LEU:H	1.94	0.44
1:D:143:ARG:HH11	3:D:604:ADP:PB	2.40	0.44
1:E:298:MET:HB2	1:E:298:MET:HE3	1.83	0.44
1:O:38:ASN:ND2	1:O:38:ASN:C	2.71	0.44
1:K:250:SER:HB2	1:K:264:PHE:HB2	1.98	0.44
1:N:41:MET:C	1:N:41:MET:SD	2.96	0.44
1:F:44:GLN:O	1:F:103:LYS:HE2	2.18	0.44
1:O:301:VAL:O	1:O:301:VAL:HG12	2.17	0.44
1:B:89:GLY:O	1:B:90:ASP:HB3	2.18	0.44
1:G:219:ALA:O	1:G:222:TRP:HB2	2.16	0.44
1:H:240:ILE:O	1:H:241:ASN:HB2	2.18	0.44
1:Q:66:LYS:NZ	1:Q:216:SER:O	2.50	0.44
1:F:58:THR:OG1	1:F:62:VAL:HB	2.18	0.44
1:K:320:ASP:OD1	1:K:330:LYS:NZ	2.43	0.44
1:E:49:LEU:HD21	1:E:99:GLU:HG2	2.00	0.44
1:C:359:GLU:O	1:C:362:GLN:N	2.50	0.44
1:P:24:LYS:HE3	1:P:25:PHE:CE2	2.53	0.44
1:I:38:ASN:HD22	1:I:38:ASN:C	2.20	0.44
1:M:285:ASN:HD22	1:M:287:ARG:N	2.14	0.44
1:P:285:ASN:HB2	1:P:291:ILE:CD1	2.45	0.44
1:N:245:HIS:C	1:N:246:ILE:HG13	2.37	0.44
1:L:362:GLN:NE2	1:L:366:ASP:OD1	2.49	0.44
1:M:139:SER:OG	3:M:613:ADP:N1	2.46	0.44
1:F:40:VAL:HG13	1:F:107:GLU:CD	2.38	0.44
1:G:314:GLU:CG	1:G:315:LYS:HD2	2.47	0.44
1:F:319:PHE:CZ	1:F:323:LEU:HD11	2.52	0.44
1:J:52:LYS:HE2	1:J:53:TYR:CZ	2.52	0.44
1:J:8:TYR:O	1:J:12:ASN:ND2	2.51	0.44
1:P:69:GLN:HB3	6:P:2360:HOH:O	2.18	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:R:176:LEU:HD21	1:R:270:GLU:HB3	2.00	0.44
1:O:25:PHE:CD1	1:P:160:ALA:HB1	2.52	0.44
1:J:139:SER:OG	3:J:610:ADP:N1	2.50	0.44
1:Q:244:ASP:OD1	1:Q:292:CYS:HB3	2.18	0.44
1:N:253:LYS:HE3	1:N:253:LYS:HB2	1.88	0.44
1:P:327:ARG:HD2	1:P:327:ARG:HA	1.81	0.44
1:D:298:MET:CE	1:D:353:LEU:HD12	2.47	0.44
1:C:105:ILE:HG12	1:C:298:MET:HE2	2.00	0.44
1:E:308:LEU:HD22	1:E:310:LEU:HD21	1.98	0.44
1:H:304:ALA:O	1:H:348:SER:HB2	2.17	0.44
1:D:85:GLY:HA2	6:D:2299:HOH:O	2.18	0.44
2:H:508:NMG:NH1	5:H:808:NO3:N	2.65	0.44
1:G:377:LYS:HE3	1:G:382:GLN:HB3	1.99	0.44
1:L:49:LEU:HD21	1:L:99:GLU:HG2	1.99	0.44
1:R:173:LEU:HD13	1:R:229:TRP:CG	2.52	0.44
1:R:229:TRP:O	1:R:230:HIS:HB3	2.18	0.44
1:R:322:MET:HG3	1:R:389:PRO:HD2	2.00	0.44
1:R:335:GLY:O	1:R:338:SER:N	2.50	0.44
1:B:208:PRO:HG3	1:B:222:TRP:NE1	2.32	0.44
1:M:191:ASN:ND2	1:M:193:LYS:N	2.61	0.44
1:L:319:PHE:CZ	1:L:323:LEU:HD11	2.53	0.44
1:K:285:ASN:HB3	1:K:288:LEU:HB2	1.98	0.44
1:D:143:ARG:HG2	1:D:144:CYS:N	2.31	0.44
1:M:313:LEU:CD2	1:M:319:PHE:CD1	3.01	0.44
1:D:300:THR:HB	1:D:302:VAL:CG2	2.48	0.44
1:I:136:TYR:CE2	1:I:372:ILE:HG23	2.53	0.44
1:I:124:HIS:CE1	1:I:262:SER:HB2	2.53	0.44
1:K:270:GLU:OE2	1:K:270:GLU:HA	2.18	0.44
1:C:221:ASP:O	1:C:224:ASP:HB2	2.18	0.44
1:E:309:ARG:NH1	1:E:342:ASP:O	2.50	0.44
1:Q:264:PHE:CE2	1:Q:268:LEU:HD22	2.53	0.44
1:I:88:PHE:HD1	1:I:292:CYS:O	2.01	0.44
1:K:357:GLU:CD	1:K:357:GLU:H	2.20	0.44
1:K:57:VAL:CG1	1:K:61:GLY:HA2	2.48	0.44
1:P:359:GLU:O	1:P:363:VAL:HG23	2.18	0.44
1:E:82:LYS:HD3	6:E:3240:HOH:O	2.17	0.44
1:P:169:VAL:O	1:P:173:LEU:HG	2.17	0.44
1:C:331:ARG:NH1	3:C:603:ADP:O2A	2.51	0.43
1:Q:308:LEU:HD13	1:Q:310:LEU:HD21	1.99	0.43
1:F:325:LYS:HD3	1:F:389:PRO:O	2.18	0.43
2:D:504:NMG:NH1	5:D:804:NO3:N	2.66	0.43
1:N:58:THR:HB	1:N:59:PRO:HD2	1.99	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:N:188:THR:HG22	1:N:223:PRO:HG2	1.98	0.43
1:Q:302:VAL:HG21	1:Q:357:GLU:HG3	1.99	0.43
1:R:34:LEU:HD13	1:R:42:ALA:HA	2.00	0.43
1:Q:50:TYR:O	1:Q:54:TRP:HB3	2.18	0.43
1:B:18:LYS:O	1:B:21:GLU:HG2	2.19	0.43
1:R:270:GLU:OE1	1:R:273:ARG:NH1	2.47	0.43
1:I:382:GLN:HB3	1:I:383:SER:H	1.57	0.43
1:M:142:ILE:CD1	1:M:261:PHE:HA	2.48	0.43
1:J:300:THR:O	1:J:302:VAL:HG23	2.18	0.43
1:K:169:VAL:O	1:K:173:LEU:HG	2.17	0.43
1:N:360:LEU:HA	1:N:360:LEU:HD23	1.85	0.43
1:H:301:VAL:HG12	1:H:301:VAL:O	2.18	0.43
1:F:137:VAL:HA	1:F:307:HIS:O	2.18	0.43
1:F:239:TRP:HB2	1:F:247:ARG:HB2	2.00	0.43
1:C:159:ARG:HD3	1:C:221:ASP:OD1	2.19	0.43
1:B:154:PRO:HA	1:B:157:MET:HG2	2.00	0.43
1:N:70:THR:HG21	1:N:212:LEU:CD1	2.48	0.43
1:C:213:LEU:HD12	1:C:218:CYS:HB2	2.00	0.43
1:M:147:SER:HB2	1:M:283:MET:HB2	2.00	0.43
1:M:40:VAL:HG12	1:M:104:CYS:SG	2.58	0.43
1:R:336:GLU:OE2	2:R:518:NMG:NE	2.49	0.43
1:R:222:TRP:CG	1:R:223:PRO:HA	2.53	0.43
1:L:320:ASP:O	1:L:323:LEU:HB2	2.18	0.43
1:Q:222:TRP:HA	1:Q:223:PRO:HA	1.83	0.43
1:B:101:PHE:O	1:B:105:ILE:HG13	2.18	0.43
1:P:168:VAL:HG13	1:P:280:HIS:CE1	2.53	0.43
1:K:357:GLU:O	1:K:361:VAL:HG23	2.18	0.43
1:L:309:ARG:HA	1:L:344:THR:HA	2.00	0.43
1:A:77:ASN:ND2	1:A:80:TYR:O	2.52	0.43
1:C:250:SER:OG	1:C:263:ARG:HD2	2.17	0.43
1:D:43:SER:HA	1:I:177:LYS:HD3	2.01	0.43
1:J:168:VAL:HG13	1:J:280:HIS:CE1	2.53	0.43
1:J:274:LEU:HA	1:J:277:GLU:HB2	2.00	0.43
1:Q:239:TRP:HB2	1:Q:247:ARG:HB2	2.00	0.43
1:C:364:LEU:HD22	1:C:368:VAL:CG2	2.47	0.43
1:I:318:ARG:HD3	1:I:388:ILE:HD13	2.00	0.43
1:D:121:ASP:O	1:D:357:GLU:HB2	2.18	0.43
1:H:18:LYS:HA	1:H:19:PRO:HD2	1.72	0.43
1:E:201:ASP:O	1:E:202:HIS:HB2	2.18	0.43
1:K:219:ALA:O	1:K:222:TRP:HB2	2.18	0.43
1:N:195:GLN:HB2	1:N:195:GLN:HE21	1.67	0.43
1:C:84:THR:HG23	1:C:108:ILE:HD11	1.99	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:153:LEU:HD21	1:D:283:MET:CE	2.45	0.43
1:N:34:LEU:HA	1:N:37:HIS:CE1	2.53	0.43
1:A:144:CYS:HB3	1:A:302:VAL:HG22	2.00	0.43
1:L:112:LYS:O	1:L:287:ARG:NH2	2.52	0.43
1:B:322:MET:CE	1:B:388:ILE:HG12	2.49	0.43
1:I:372:ILE:HG22	1:I:376:LYS:HE2	1.99	0.43
1:Q:49:LEU:HD11	1:Q:103:LYS:HE2	2.00	0.43
1:C:212:LEU:O	1:C:216:SER:HB3	2.17	0.43
1:B:140:CYS:SG	1:B:306:VAL:HG12	2.59	0.43
1:E:305:SER:CB	1:E:348:SER:HB3	2.47	0.43
1:A:237:LEU:HD12	1:A:237:LEU:N	2.33	0.43
1:Q:153:LEU:HB3	1:Q:154:PRO:HD2	2.00	0.43
1:K:228:ILE:HD11	1:K:237:LEU:HD23	2.01	0.43
1:A:314:GLU:HG3	1:A:315:LYS:HD2	2.01	0.43
1:C:111:PHE:HE2	1:C:287:ARG:NH2	2.17	0.43
1:D:372:ILE:HG22	1:D:376:LYS:HE2	2.00	0.43
1:A:49:LEU:HD21	1:A:99:GLU:HG2	2.01	0.43
1:E:384:ILE:HA	1:E:387:MET:HG3	1.99	0.43
1:Q:199:ILE:HG12	1:Q:205:PHE:O	2.19	0.43
1:G:40:VAL:HB	1:G:84:THR:HA	1.99	0.43
1:G:66:LYS:NZ	1:G:216:SER:O	2.52	0.43
1:Q:346:ASP:C	1:Q:346:ASP:OD1	2.57	0.43
1:L:199:ILE:HD13	1:L:206:GLU:HA	2.00	0.43
1:R:298:MET:HG2	6:R:2089:HOH:O	2.17	0.43
1:F:24:LYS:HE3	1:F:25:PHE:CE2	2.52	0.43
1:N:248:VAL:C	1:N:249:ILE:HG13	2.39	0.43
1:M:108:ILE:HG21	1:M:296:THR:HG22	1.99	0.43
1:N:147:SER:HB3	1:N:283:MET:HE3	2.00	0.43
1:D:18:LYS:HA	1:D:19:PRO:HD2	1.84	0.43
1:L:59:PRO:HD2	1:L:92:TYR:CG	2.54	0.43
1:B:366:ASP:HB3	1:C:126:LYS:HD2	1.99	0.43
1:H:285:ASN:HB3	1:H:288:LEU:HB2	1.99	0.43
1:K:38:ASN:ND2	1:K:38:ASN:C	2.71	0.43
1:N:57:VAL:CG1	1:N:58:THR:N	2.81	0.43
1:G:328:LEU:HD22	1:G:364:LEU:HD23	2.01	0.43
1:J:154:PRO:HD3	1:J:245:HIS:NE2	2.33	0.43
1:N:18:LYS:HB2	1:N:21:GLU:CD	2.38	0.43
1:O:285:ASN:ND2	1:O:288:LEU:HG	2.33	0.43
1:R:91:GLU:HG3	1:R:283:MET:CG	2.48	0.43
1:I:159:ARG:NH2	1:J:65:ASP:OD1	2.45	0.43
1:E:294:CYS:HA	1:E:295:PRO:HD3	1.91	0.43
1:F:326:LEU:O	1:F:327:ARG:HB2	2.18	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:O:154:PRO:HG2	1:O:243:GLU:O	2.17	0.43
1:I:168:VAL:HG12	1:I:169:VAL:N	2.33	0.43
1:C:268:LEU:O	1:C:272:GLU:HG3	2.19	0.43
1:H:237:LEU:N	1:H:237:LEU:HD12	2.34	0.43
1:J:94:TYR:CZ	1:J:288:LEU:HD11	2.54	0.43
1:F:222:TRP:HA	1:F:223:PRO:HA	1.82	0.43
1:F:132:PHE:CD1	1:F:137:VAL:HG21	2.54	0.43
1:D:297:ASN:O	1:D:301:VAL:HG13	2.19	0.43
1:N:141:ARG:HG3	1:N:251:MET:HB3	2.00	0.43
1:J:106:GLU:HG3	1:J:112:LYS:HA	2.01	0.43
1:R:331:ARG:NH1	3:R:618:ADP:O2A	2.52	0.43
1:R:176:LEU:HA	1:R:176:LEU:HD23	1.78	0.43
1:R:236:PHE:HB2	1:R:263:ARG:HD3	2.00	0.43
1:N:13:ARG:NH1	1:N:156:ALA:O	2.52	0.43
1:O:340:ALA:HB2	1:O:345:TYR:CE2	2.54	0.43
1:B:34:LEU:HD13	1:B:42:ALA:HA	1.99	0.43
1:J:232:ASN:OD1	1:J:232:ASN:N	2.52	0.43
1:E:208:PRO:HG3	1:E:222:TRP:CG	2.54	0.42
1:M:331:ARG:HB2	1:M:346:ASP:HB3	2.00	0.42
1:F:327:ARG:NH1	6:F:1492:HOH:O	2.52	0.42
1:L:153:LEU:HB3	1:L:154:PRO:HD2	2.01	0.42
1:H:90:ASP:HB2	6:H:2395:HOH:O	2.18	0.42
1:K:192:GLU:O	1:K:196:GLU:HG3	2.19	0.42
1:L:368:VAL:HA	1:L:371:LEU:HD12	2.01	0.42
1:B:271:VAL:O	1:B:275:MET:HG2	2.19	0.42
1:C:151:VAL:HG13	1:C:161:GLU:HB3	2.00	0.42
1:M:290:TYR:HB3	6:M:2237:HOH:O	2.17	0.42
1:D:358:ARG:HH21	1:D:359:GLU:HG3	1.82	0.42
1:H:172:ALA:C	1:H:174:GLY:H	2.23	0.42
1:I:278:CYS:HB3	1:I:280:HIS:CE1	2.54	0.42
1:D:14:VAL:HG23	6:D:1559:HOH:O	2.18	0.42
1:M:144:CYS:HA	1:M:301:VAL:O	2.18	0.42
1:R:308:LEU:HD13	1:R:310:LEU:CG	2.49	0.42
1:E:346:ASP:OD1	1:E:346:ASP:C	2.58	0.42
1:B:105:ILE:CG2	1:B:298:MET:HE1	2.46	0.42
1:D:132:PHE:CE1	1:D:257:LEU:HD12	2.51	0.42
1:P:20:TRP:HB3	1:P:54:TRP:CH2	2.54	0.42
1:N:184:TYR:CD2	1:N:186:PRO:HD3	2.54	0.42
1:O:136:TYR:O	1:O:308:LEU:HA	2.19	0.42
1:O:207:LYS:HB3	1:O:208:PRO:HD2	2.02	0.42
1:E:158:SER:CB	1:F:19:PRO:HG3	2.50	0.42
1:A:340:ALA:HB2	1:A:345:TYR:CD2	2.54	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:N:155:PRO:HG3	1:N:218:CYS:SG	2.59	0.42
1:B:241:ASN:HA	1:B:244:ASP:O	2.20	0.42
1:N:304:ALA:O	1:N:348:SER:HB2	2.19	0.42
1:N:47:LYS:HG3	6:N:1687:HOH:O	2.19	0.42
1:H:190:MET:SD	1:H:195:GLN:HB2	2.58	0.42
1:M:223:PRO:O	1:M:224:ASP:C	2.57	0.42
1:B:307:HIS:CE1	3:B:602:ADP:C2	3.08	0.42
1:E:141:ARG:NE	6:E:1661:HOH:O	2.45	0.42
1:D:205:PHE:HD2	1:D:239:TRP:CD2	2.36	0.42
1:F:298:MET:HE3	1:F:298:MET:HB2	1.80	0.42
1:B:83:LYS:NZ	1:B:336:GLU:OE2	2.53	0.42
1:M:360:LEU:O	1:M:363:VAL:HB	2.19	0.42
1:L:305:SER:CB	1:L:348:SER:HB3	2.49	0.42
1:Q:318:ARG:HD3	1:Q:388:ILE:CD1	2.49	0.42
1:J:8:TYR:HD2	1:J:11:LYS:HZ3	1.67	0.42
1:P:80:TYR:CD1	1:P:330:LYS:HG2	2.54	0.42
1:M:183:LYS:HG2	1:M:184:TYR:N	2.34	0.42
1:B:126:LYS:HB2	1:B:358:ARG:HD3	2.02	0.42
1:C:126:LYS:HB2	1:C:358:ARG:CD	2.29	0.42
1:P:285:ASN:HD22	1:P:288:LEU:N	2.15	0.42
1:E:112:LYS:HB3	1:E:113:PRO:HD2	2.02	0.42
1:E:300:THR:HB	1:E:302:VAL:HG23	2.00	0.42
1:R:340:ALA:HB2	1:R:345:TYR:CE2	2.54	0.42
1:Q:149:LYS:N	1:Q:281:GLY:O	2.52	0.42
1:K:154:PRO:HG2	1:K:243:GLU:O	2.18	0.42
1:L:59:PRO:HD2	1:L:92:TYR:CD1	2.54	0.42
1:D:40:VAL:HG23	1:D:84:THR:HA	2.01	0.42
1:L:357:GLU:N	1:L:357:GLU:OE1	2.40	0.42
1:M:285:ASN:OD1	1:M:288:LEU:HD12	2.20	0.42
1:D:297:ASN:HB3	1:D:301:VAL:CG1	2.47	0.42
1:N:173:LEU:HD13	1:N:229:TRP:CG	2.55	0.42
1:F:143:ARG:HH22	1:F:297:ASN:CG	2.22	0.42
1:B:152:CYS:HB2	1:B:161:GLU:CD	2.40	0.42
1:R:184:TYR:CZ	1:R:227:GLY:HA3	2.54	0.42
1:E:143:ARG:HD3	1:E:303:ARG:HB3	2.00	0.42
1:D:79:PHE:HB3	6:D:2775:HOH:O	2.20	0.42
1:F:327:ARG:O	1:F:350:TRP:HB3	2.20	0.42
1:Q:177:LYS:HD3	6:Q:3221:HOH:O	2.18	0.42
1:J:290:TYR:O	1:J:298:MET:HA	2.19	0.42
1:D:73:ASP:C	1:D:75:PRO:HD3	2.40	0.42
1:P:84:THR:HB	6:P:2550:HOH:O	2.18	0.42
1:G:187:LEU:HD11	1:G:195:GLN:HG3	2.02	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:285:ASN:ND2	1:B:287:ARG:H	2.18	0.42
1:Q:301:VAL:HG12	1:Q:301:VAL:O	2.20	0.42
1:O:141:ARG:HD2	3:O:615:ADP:C4	2.55	0.42
1:R:142:ILE:HD12	1:R:261:PHE:HA	2.02	0.42
1:G:300:THR:C	1:G:301:VAL:HG23	2.40	0.42
1:L:358:ARG:HB3	1:L:358:ARG:HE	1.53	0.42
1:D:79:PHE:CE2	1:D:337:SER:HB2	2.55	0.42
1:B:244:ASP:OD1	1:B:292:CYS:HB3	2.20	0.42
1:I:213:LEU:HD12	1:I:218:CYS:HB2	2.02	0.42
1:Q:316:HIS:HA	1:Q:317:PRO:HD2	1.86	0.42
1:C:273:ARG:O	1:C:277:GLU:HB2	2.20	0.42
1:L:295:PRO:O	1:L:298:MET:HE1	2.20	0.42
1:L:246:ILE:O	1:L:247:ARG:HG2	2.20	0.42
1:G:364:LEU:O	1:G:368:VAL:HG23	2.19	0.42
1:F:94:TYR:CZ	1:F:98:LYS:HG3	2.55	0.42
1:R:313:LEU:HD23	1:R:316:HIS:CB	2.50	0.42
1:L:112:LYS:HB3	1:L:113:PRO:CD	2.50	0.42
1:R:184:TYR:CE1	1:R:227:GLY:HA3	2.55	0.42
1:O:136:TYR:HB3	1:O:308:LEU:HD21	2.01	0.42
1:O:105:ILE:HG12	1:O:298:MET:CE	2.50	0.42
1:H:70:THR:O	1:H:74:ASN:ND2	2.53	0.42
1:K:26:LYS:O	1:K:29:ASP:HB2	2.19	0.42
1:I:79:PHE:HB3	6:I:1411:HOH:O	2.19	0.42
1:A:157:MET:HE2	1:A:161:GLU:HB2	2.01	0.42
1:B:44:GLN:HG3	1:B:103:LYS:O	2.20	0.42
1:I:138:LYS:O	1:I:139:SER:HB3	2.20	0.42
1:D:327:ARG:HA	6:D:1981:HOH:O	2.20	0.42
1:B:367:GLY:O	1:B:371:LEU:HG	2.19	0.42
1:E:162:ARG:HG2	1:E:241:ASN:ND2	2.34	0.42
1:J:360:LEU:HD23	1:J:360:LEU:HA	1.87	0.42
1:D:360:LEU:HA	1:D:360:LEU:HD23	1.87	0.42
1:M:327:ARG:HD2	1:M:327:ARG:HA	1.90	0.42
1:B:202:HIS:HB3	3:B:602:ADP:H1'	2.02	0.42
1:D:8:TYR:HA	1:D:11:LYS:HZ3	1.84	0.42
1:I:49:LEU:HA	1:I:49:LEU:HD23	1.93	0.42
1:M:346:ASP:C	1:M:346:ASP:OD1	2.58	0.42
1:K:205:PHE:HD2	1:K:239:TRP:CG	2.37	0.42
1:Q:79:PHE:CD2	1:Q:337:SER:HA	2.55	0.42
1:J:8:TYR:CD2	1:J:11:LYS:HE2	2.54	0.42
3:J:610:ADP:H8	3:J:610:ADP:H5'1	1.85	0.42
1:R:18:LYS:HB2	1:R:21:GLU:CD	2.40	0.42
1:L:192:GLU:O	1:L:193:LYS:C	2.58	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:J:309:ARG:NH1	1:J:342:ASP:OD1	2.53	0.42
1:G:94:TYR:CZ	1:G:288:LEU:HD11	2.55	0.42
1:J:159:ARG:HG3	6:J:1493:HOH:O	2.18	0.42
1:D:250:SER:OG	1:D:260:VAL:HG13	2.19	0.42
1:D:285:ASN:ND2	1:D:287:ARG:H	2.18	0.42
1:K:313:LEU:HD12	1:K:374:CYS:HB2	2.01	0.42
1:F:117:HIS:HB2	1:F:353:LEU:HD21	2.02	0.42
1:F:112:LYS:O	1:F:115:ASP:N	2.40	0.42
1:I:226:ARG:CG	1:I:241:ASN:O	2.68	0.42
1:B:274:LEU:HD23	1:B:274:LEU:HA	1.91	0.42
1:D:358:ARG:NH2	6:D:1318:HOH:O	2.52	0.42
1:H:195:GLN:O	1:H:199:ILE:HG13	2.20	0.42
1:J:109:HIS:C	1:J:111:PHE:N	2.71	0.42
6:Q:1605:HOH:O	1:R:36:LYS:HD2	2.19	0.42
1:F:273:ARG:O	1:F:277:GLU:HB2	2.20	0.42
1:J:238:VAL:HA	1:J:247:ARG:O	2.20	0.42
1:J:270:GLU:OE2	1:J:270:GLU:HA	2.20	0.42
1:R:345:TYR:CD1	1:R:345:TYR:N	2.87	0.41
1:I:144:CYS:HB3	1:I:264:PHE:HZ	1.85	0.41
1:G:388:ILE:HA	1:G:389:PRO:HD3	1.82	0.41
1:R:143:ARG:NH2	1:R:297:ASN:OD1	2.42	0.41
1:O:74:ASN:OD1	1:O:211:ALA:HB1	2.20	0.41
1:Q:69:GLN:HE21	1:Q:73:ASP:CG	2.24	0.41
1:R:69:GLN:HE21	1:R:73:ASP:CG	2.23	0.41
1:N:191:ASN:ND2	1:N:192:GLU:N	2.68	0.41
1:C:94:TYR:CZ	1:C:288:LEU:HD11	2.55	0.41
1:N:141:ARG:HD3	3:N:614:ADP:C5	2.55	0.41
1:H:106:GLU:OE2	1:H:112:LYS:HE2	2.19	0.41
1:K:240:ILE:O	1:K:241:ASN:HB2	2.20	0.41
1:A:58:THR:HB	1:A:59:PRO:HD2	2.02	0.41
1:B:157:MET:HE2	1:B:161:GLU:HB3	2.02	0.41
1:Q:298:MET:HB2	1:Q:298:MET:HE3	1.92	0.41
1:R:18:LYS:O	1:R:21:GLU:HG2	2.20	0.41
1:L:338:SER:O	1:L:339:LEU:HD23	2.20	0.41
1:Q:213:LEU:HD12	1:Q:218:CYS:HB2	2.03	0.41
1:I:172:ALA:O	1:I:274:LEU:HD13	2.19	0.41
1:L:88:PHE:HE2	1:L:101:PHE:CD2	2.38	0.41
1:P:143:ARG:HG3	6:P:1051:HOH:O	2.20	0.41
1:L:274:LEU:O	1:L:277:GLU:N	2.53	0.41
1:I:151:VAL:CG1	1:I:152:CYS:N	2.83	0.41
3:R:618:ADP:H2'	6:R:1004:HOH:O	2.21	0.41
1:P:229:TRP:CE3	1:P:230:HIS:HA	2.55	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:R:277:GLU:CG	1:R:277:GLU:O	2.69	0.41
1:J:37:HIS:HD2	1:J:71:GLY:O	2.03	0.41
1:N:236:PHE:CZ	1:N:267:GLY:HA3	2.55	0.41
1:C:89:GLY:HA2	1:C:155:PRO:HG2	2.01	0.41
1:N:24:LYS:HE3	1:N:25:PHE:CE2	2.54	0.41
1:L:237:LEU:HD12	1:L:237:LEU:N	2.35	0.41
1:B:287:ARG:HD3	1:B:287:ARG:HH11	1.74	0.41
1:L:314:GLU:CG	1:L:315:LYS:HD2	2.49	0.41
1:H:187:LEU:HB3	1:H:223:PRO:HB2	2.02	0.41
1:K:34:LEU:HA	1:K:37:HIS:CE1	2.55	0.41
1:B:49:LEU:HD13	1:B:100:PHE:HA	2.02	0.41
1:Q:294:CYS:HB2	6:Q:1771:HOH:O	2.19	0.41
1:Q:112:LYS:O	1:Q:115:ASP:HB2	2.20	0.41
1:K:342:ASP:O	1:K:343:SER:HB2	2.21	0.41
1:N:313:LEU:HA	1:N:378:LEU:HD12	2.01	0.41
1:R:77:ASN:ND2	1:R:83:LYS:HE2	2.35	0.41
1:H:384:ILE:O	1:H:388:ILE:HG13	2.20	0.41
1:G:242:GLU:CG	1:G:243:GLU:H	2.33	0.41
3:M:613:ADP:H2'	6:M:1458:HOH:O	2.21	0.41
1:E:154:PRO:HA	1:E:157:MET:SD	2.60	0.41
1:K:58:THR:C	1:K:60:ASN:N	2.74	0.41
1:Q:266:ARG:HA	6:Q:2161:HOH:O	2.19	0.41
1:G:270:GLU:O	1:G:274:LEU:HG	2.20	0.41
1:B:142:ILE:HG13	1:B:260:VAL:CG1	2.51	0.41
1:N:182:GLY:HA3	1:N:230:HIS:O	2.20	0.41
1:P:88:PHE:CE1	1:P:295:PRO:HG3	2.55	0.41
1:M:203:PHE:CE2	1:M:234:LYS:HE3	2.56	0.41
1:H:50:TYR:O	1:H:54:TRP:HB3	2.20	0.41
1:L:144:CYS:SG	1:L:146:ARG:NH1	2.93	0.41
1:O:84:THR:OG1	2:O:515:NMG:O2	2.22	0.41
1:A:265:ALA:O	1:A:269:LEU:HG	2.20	0.41
1:B:151:VAL:CG1	1:B:157:MET:HE3	2.51	0.41
1:D:73:ASP:O	1:D:75:PRO:HD3	2.20	0.41
1:D:367:GLY:O	1:D:371:LEU:HG	2.21	0.41
1:A:50:TYR:O	1:A:54:TRP:HB3	2.21	0.41
1:G:111:PHE:HE2	1:G:287:ARG:HH21	1.67	0.41
1:A:284:HIS:CD2	1:A:285:ASN:O	2.74	0.41
1:F:157:MET:HB2	1:F:161:GLU:OE1	2.19	0.41
1:F:298:MET:HE1	1:F:353:LEU:HD12	2.02	0.41
1:N:18:LYS:HB2	1:N:21:GLU:HG2	2.03	0.41
1:G:38:ASN:HD21	1:G:82:LYS:HE3	1.84	0.41
1:Q:319:PHE:O	1:Q:323:LEU:HG	2.20	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:388:ILE:HA	1:F:389:PRO:HD3	1.88	0.41
1:M:142:ILE:HD12	1:M:261:PHE:HA	2.02	0.41
1:P:88:PHE:O	1:P:153:LEU:HD12	2.20	0.41
1:P:58:THR:O	1:P:60:ASN:N	2.54	0.41
1:M:154:PRO:N	1:M:155:PRO:HD2	2.35	0.41
1:H:83:LYS:NZ	1:H:336:GLU:OE2	2.49	0.41
1:H:249:ILE:HD13	6:H:2151:HOH:O	2.20	0.41
1:Q:207:LYS:HB3	1:Q:208:PRO:HD2	2.03	0.41
1:K:117:HIS:ND1	1:K:118:PRO:HD2	2.35	0.41
1:F:199:ILE:HD13	1:F:206:GLU:HA	2.02	0.41
1:P:141:ARG:NH1	3:P:616:ADP:O2B	2.51	0.41
1:E:298:MET:HE1	1:E:353:LEU:HD12	2.00	0.41
1:G:313:LEU:C	1:G:313:LEU:HD23	2.41	0.41
1:F:196:GLU:O	1:F:200:GLU:HB2	2.20	0.41
1:L:112:LYS:O	1:L:115:ASP:HB2	2.21	0.41
1:P:236:PHE:CE1	1:P:267:GLY:HA3	2.55	0.41
1:D:250:SER:OG	1:D:263:ARG:NH1	2.51	0.41
1:A:71:GLY:N	1:A:85:GLY:O	2.54	0.41
1:I:74:ASN:HA	1:I:75:PRO:HD2	1.84	0.41
1:G:304:ALA:O	1:G:348:SER:HB2	2.21	0.41
1:J:83:LYS:NZ	1:J:336:GLU:HG2	2.35	0.41
1:H:179:ASP:CG	1:H:266:ARG:HH12	2.24	0.41
1:D:285:ASN:CB	1:D:288:LEU:HB2	2.51	0.41
1:L:96:CYS:HB3	1:L:97:TYR:CE2	2.56	0.41
1:F:220:ARG:C	1:F:222:TRP:H	2.24	0.41
1:I:377:LYS:HB2	1:I:384:ILE:CG2	2.51	0.41
1:D:139:SER:HB2	1:D:252:GLN:O	2.20	0.41
1:C:372:ILE:CG2	1:C:376:LYS:HE2	2.50	0.41
1:Q:352:ARG:HG2	1:Q:352:ARG:NH1	2.34	0.41
1:F:38:ASN:HB2	1:K:177:LYS:HD2	2.03	0.41
1:I:313:LEU:HD22	1:I:319:PHE:CD1	2.56	0.41
1:B:111:PHE:CG	1:B:353:LEU:HD13	2.55	0.41
1:N:119:ALA:HA	1:N:120:PRO:HD3	1.95	0.41
1:I:66:LYS:NZ	1:I:155:PRO:O	2.54	0.41
1:E:328:LEU:HD11	1:E:367:GLY:HA3	2.01	0.41
1:D:57:VAL:HG12	1:D:58:THR:N	2.35	0.41
1:H:252:GLN:OE1	1:H:263:ARG:NH2	2.53	0.41
1:P:325:LYS:HD3	1:P:389:PRO:HB2	2.02	0.41
1:C:267:GLY:O	1:C:270:GLU:HB2	2.21	0.41
1:O:204:LEU:CD1	1:O:228:ILE:HB	2.51	0.41
1:A:141:ARG:HH21	1:A:249:ILE:HD13	1.86	0.41
1:B:326:LEU:HB3	6:B:1699:HOH:O	2.20	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:I:133:GLU:HB2	6:I:1271:HOH:O	2.20	0.41
1:Q:117:HIS:HA	1:Q:118:PRO:HD2	1.86	0.41
1:M:58:THR:HB	1:M:59:PRO:HD2	2.03	0.41
1:R:323:LEU:HD13	1:R:330:LYS:HB2	2.03	0.41
1:E:195:GLN:HB2	1:E:195:GLN:HE21	1.62	0.41
1:H:382:GLN:HE21	1:H:382:GLN:HB2	1.70	0.41
1:L:105:ILE:HG12	1:L:298:MET:CE	2.51	0.41
1:A:168:VAL:HG13	1:A:280:HIS:CE1	2.56	0.41
1:O:137:VAL:CG1	1:O:255:GLY:HA2	2.51	0.41
1:M:298:MET:HG2	6:M:2679:HOH:O	2.21	0.41
1:P:183:LYS:HG2	1:P:184:TYR:N	2.36	0.41
1:L:38:ASN:N	1:L:75:PRO:O	2.50	0.41
1:G:98:LYS:HE3	1:G:102:ASP:OD2	2.20	0.41
1:H:352:ARG:NH1	1:H:352:ARG:HG3	2.35	0.40
1:I:384:ILE:CB	1:I:387:MET:HG3	2.52	0.40
1:K:144:CYS:SG	1:K:264:PHE:HZ	2.44	0.40
1:I:340:ALA:HB2	1:I:345:TYR:CE2	2.55	0.40
1:G:56:LYS:HE2	1:G:96:CYS:SG	2.62	0.40
1:L:137:VAL:HG12	1:L:255:GLY:HA2	2.03	0.40
1:C:206:GLU:HG3	6:C:2835:HOH:O	2.21	0.40
1:M:357:GLU:O	1:M:361:VAL:HG23	2.21	0.40
1:R:326:LEU:HB3	6:R:1273:HOH:O	2.21	0.40
1:L:290:TYR:O	1:L:298:MET:HA	2.21	0.40
1:L:294:CYS:HA	1:L:295:PRO:HD3	1.84	0.40
1:A:331:ARG:NH1	3:A:601:ADP:O2A	2.50	0.40
1:J:314:GLU:CG	1:J:315:LYS:HD2	2.51	0.40
1:E:208:PRO:HD3	1:E:222:TRP:CE2	2.56	0.40
1:F:135:LYS:HD3	1:F:136:TYR:CE1	2.57	0.40
1:C:151:VAL:HG12	1:C:152:CYS:O	2.21	0.40
1:N:20:TRP:HB3	1:N:54:TRP:CZ2	2.56	0.40
1:J:336:GLU:OE2	2:J:510:NMG:NE	2.27	0.40
1:I:154:PRO:N	1:I:155:PRO:HD2	2.36	0.40
1:B:187:LEU:HD11	1:B:204:LEU:HD21	2.04	0.40
1:A:132:PHE:O	1:A:255:GLY:HA3	2.20	0.40
1:J:133:GLU:HG3	6:J:1050:HOH:O	2.21	0.40
1:J:367:GLY:O	1:J:371:LEU:HG	2.21	0.40
1:P:352:ARG:HH11	1:P:352:ARG:HG2	1.86	0.40
1:D:285:ASN:ND2	1:D:288:LEU:N	2.57	0.40
1:P:284:HIS:CD2	1:P:285:ASN:O	2.74	0.40
1:J:322:MET:HE2	1:J:388:ILE:HG12	2.04	0.40
1:P:18:LYS:HB2	1:P:21:GLU:HG2	2.03	0.40
1:L:47:LYS:O	1:L:51:GLU:HB2	2.22	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:L:242:GLU:OE1	1:L:243:GLU:N	2.50	0.40
1:M:318:ARG:NH1	1:M:385:ASP:OD2	2.54	0.40
1:B:364:LEU:O	1:B:364:LEU:HD22	2.21	0.40
1:F:316:HIS:HA	1:F:317:PRO:HD2	1.87	0.40
1:O:353:LEU:HD22	1:O:354:GLY:N	2.37	0.40
1:O:74:ASN:HA	1:O:75:PRO:HD2	1.84	0.40
1:P:83:LYS:NZ	1:P:336:GLU:OE2	2.54	0.40
1:J:8:TYR:HA	1:J:11:LYS:HZ3	1.87	0.40
1:G:70:THR:HB	1:G:216:SER:HB3	2.03	0.40
1:I:309:ARG:NH1	6:I:2748:HOH:O	2.48	0.40
1:A:105:ILE:HG12	1:A:298:MET:CE	2.52	0.40
1:E:385:ASP:HA	1:E:388:ILE:HD12	2.03	0.40
1:O:236:PHE:CZ	1:O:267:GLY:HA3	2.56	0.40
1:N:40:VAL:O	1:N:41:MET:C	2.60	0.40
1:D:320:ASP:N	6:D:2678:HOH:O	2.51	0.40
1:R:294:CYS:O	1:R:297:ASN:HB2	2.22	0.40
1:K:70:THR:HG21	1:K:212:LEU:HD12	2.02	0.40
1:H:83:LYS:HB2	6:H:3162:HOH:O	2.21	0.40
1:Q:117:HIS:HE1	1:Q:300:THR:HG23	1.87	0.40
1:C:40:VAL:N	1:C:82:LYS:HE2	2.36	0.40
1:E:68:ILE:O	1:E:72:VAL:HG23	2.21	0.40
1:D:331:ARG:HB2	1:D:346:ASP:HB3	2.04	0.40
1:L:45:LEU:HD12	1:L:45:LEU:HA	1.92	0.40
1:D:287:ARG:NH1	6:D:1795:HOH:O	2.55	0.40
1:N:364:LEU:HD22	1:N:368:VAL:HG23	2.02	0.40
1:H:247:ARG:HD2	6:H:1174:HOH:O	2.22	0.40
1:H:352:ARG:HH11	1:H:352:ARG:HG3	1.86	0.40
1:L:141:ARG:HH21	1:L:249:ILE:HD13	1.87	0.40
1:B:312:PHE:CE2	1:B:379:GLU:HA	2.56	0.40
1:Q:74:ASN:HA	1:Q:75:PRO:HD2	1.95	0.40
1:Q:110:HIS:NE2	1:Q:327:ARG:NH1	2.69	0.40
1:C:222:TRP:CD1	1:C:223:PRO:HB3	2.57	0.40
1:D:154:PRO:HA	1:D:157:MET:SD	2.62	0.40
1:C:327:ARG:HD2	1:C:327:ARG:HA	1.84	0.40
1:Q:388:ILE:HA	1:Q:389:PRO:HD3	1.83	0.40
1:D:12:ASN:OD1	1:D:18:LYS:HE3	2.21	0.40
1:D:18:LYS:O	1:D:21:GLU:HG2	2.20	0.40
1:J:326:LEU:HD13	1:J:367:GLY:CA	2.51	0.40
1:C:294:CYS:HA	1:C:295:PRO:HD3	1.92	0.40
1:O:58:THR:HG23	1:O:62:VAL:O	2.21	0.40
1:F:252:GLN:HG2	1:F:260:VAL:CG2	2.51	0.40
1:G:119:ALA:HA	1:G:120:PRO:HD3	1.96	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:Q:165:VAL:O	1:Q:169:VAL:HG23	2.21	0.40
1:F:312:PHE:CZ	1:F:379:GLU:HG3	2.57	0.40
1:G:355:LYS:HB2	1:G:360:LEU:HD21	2.03	0.40
1:M:36:LYS:HG3	6:M:2755:HOH:O	2.21	0.40
1:P:127:LEU:HD12	1:P:362:GLN:OE1	2.21	0.40
1:J:311:ALA:HB3	6:J:1482:HOH:O	2.22	0.40
1:F:187:LEU:HA	1:F:187:LEU:HD12	1.66	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	A	365/390 (94%)	337 (92%)	23 (6%)	5 (1%)	16	15
1	B	386/390 (99%)	358 (93%)	24 (6%)	4 (1%)	22	23
1	C	365/390 (94%)	341 (93%)	23 (6%)	1 (0%)	50	60
1	D	383/390 (98%)	351 (92%)	29 (8%)	3 (1%)	27	30
1	E	365/390 (94%)	337 (92%)	25 (7%)	3 (1%)	27	30
1	F	380/390 (97%)	344 (90%)	33 (9%)	3 (1%)	27	30
1	G	365/390 (94%)	334 (92%)	29 (8%)	2 (0%)	38	45
1	H	380/390 (97%)	353 (93%)	23 (6%)	4 (1%)	21	21
1	I	365/390 (94%)	342 (94%)	22 (6%)	1 (0%)	50	60
1	J	383/390 (98%)	355 (93%)	26 (7%)	2 (0%)	38	45
1	K	365/390 (94%)	341 (93%)	23 (6%)	1 (0%)	50	60
1	L	379/390 (97%)	331 (87%)	40 (11%)	8 (2%)	11	8
1	M	365/390 (94%)	345 (94%)	19 (5%)	1 (0%)	50	60
1	N	380/390 (97%)	349 (92%)	26 (7%)	5 (1%)	18	17
1	O	365/390 (94%)	344 (94%)	19 (5%)	2 (0%)	38	45
1	P	380/390 (97%)	348 (92%)	29 (8%)	3 (1%)	27	30

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Q	364/390 (93%)	342 (94%)	20 (6%)	2 (0%)	38	45
1	R	379/390 (97%)	353 (93%)	24 (6%)	2 (0%)	38	45
All	All	6714/7020 (96%)	6205 (92%)	457 (7%)	52 (1%)	27	30

All (52) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	242	GLU
1	H	242	GLU
1	L	206	GLU
1	Q	242	GLU
1	A	301	VAL
1	B	385	ASP
1	D	115	ASP
1	F	220	ARG
1	J	94	TYR
1	L	283	MET
1	L	381	GLY
1	P	242	GLU
1	A	202	HIS
1	A	342	ASP
1	D	17	SER
1	F	221	ASP
1	J	241	ASN
1	L	133	GLU
1	L	134	ASP
1	L	242	GLU
1	N	152	CYS
1	N	186	PRO
1	N	242	GLU
1	O	242	GLU
1	B	13	ARG
1	B	242	GLU
1	E	220	ARG
1	G	301	VAL
1	L	126	LYS
1	R	208	PRO
1	A	242	GLU
1	H	208	PRO
1	H	365	VAL
1	P	59	PRO

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Mol	Chain	Res	Type
1	Q	299	GLY
1	C	283	MET
1	E	242	GLU
1	E	301	VAL
1	F	301	VAL
1	L	301	VAL
1	N	93	SER
1	N	158	SER
1	M	301	VAL
1	P	301	VAL
1	O	301	VAL
1	D	301	VAL
1	I	301	VAL
1	K	59	PRO
1	R	301	VAL
1	A	168	VAL
1	B	301	VAL
1	H	301	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	A	316/335 (94%)	301 (95%)	15 (5%)	36	47
1	B	334/335 (100%)	317 (95%)	17 (5%)	33	43
1	C	316/335 (94%)	303 (96%)	13 (4%)	41	55
1	D	332/335 (99%)	313 (94%)	19 (6%)	29	37
1	E	316/335 (94%)	299 (95%)	17 (5%)	31	40
1	F	329/335 (98%)	311 (94%)	18 (6%)	30	39
1	G	316/335 (94%)	301 (95%)	15 (5%)	36	47
1	H	329/335 (98%)	315 (96%)	14 (4%)	40	52
1	I	316/335 (94%)	299 (95%)	17 (5%)	31	40
1	J	332/335 (99%)	315 (95%)	17 (5%)	33	43
1	K	316/335 (94%)	299 (95%)	17 (5%)	31	40

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	L	328/335 (98%)	310 (94%)	18 (6%)	30	39
1	M	316/335 (94%)	300 (95%)	16 (5%)	33	43
1	N	329/335 (98%)	310 (94%)	19 (6%)	28	36
1	O	316/335 (94%)	305 (96%)	11 (4%)	48	63
1	P	329/335 (98%)	316 (96%)	13 (4%)	42	56
1	Q	315/335 (94%)	296 (94%)	19 (6%)	27	35
1	R	328/335 (98%)	311 (95%)	17 (5%)	32	42
All	All	5813/6030 (96%)	5521 (95%)	292 (5%)	34	45

All (292) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	ASN
1	A	54	TRP
1	A	91	GLU
1	A	143	ARG
1	A	149	LYS
1	A	195	GLN
1	A	200	GLU
1	A	237	LEU
1	A	257	LEU
1	A	286	ASP
1	A	308	LEU
1	A	333	THR
1	A	346	ASP
1	A	353	LEU
1	A	382	GLN
1	B	6	GLN
1	B	7	ASP
1	B	22	SER
1	B	26	LYS
1	B	35	SER
1	B	54	TRP
1	B	66	LYS
1	B	152	CYS
1	B	191	ASN
1	B	223	PRO
1	B	257	LEU
1	B	266	ARG
1	B	291	ILE

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Mol	Chain	Res	Type
1	B	308	LEU
1	B	313	LEU
1	B	353	LEU
1	B	364	LEU
1	C	91	GLU
1	C	143	ARG
1	C	257	LEU
1	C	285	ASN
1	C	286	ASP
1	C	308	LEU
1	C	313	LEU
1	C	333	THR
1	C	342	ASP
1	C	353	LEU
1	C	364	LEU
1	C	383	SER
1	C	387	MET
1	D	6	GLN
1	D	22	SER
1	D	26	LYS
1	D	54	TRP
1	D	66	LYS
1	D	110	HIS
1	D	143	ARG
1	D	151	VAL
1	D	168	VAL
1	D	191	ASN
1	D	195	GLN
1	D	213	LEU
1	D	226	ARG
1	D	257	LEU
1	D	308	LEU
1	D	353	LEU
1	D	364	LEU
1	D	382	GLN
1	D	387	MET
1	E	35	SER
1	E	38	ASN
1	E	54	TRP
1	E	103	LYS
1	E	134	ASP
1	E	143	ARG

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Mol	Chain	Res	Type
1	E	200	GLU
1	E	257	LEU
1	E	308	LEU
1	E	313	LEU
1	E	333	THR
1	E	353	LEU
1	E	364	LEU
1	E	382	GLN
1	E	383	SER
1	E	385	ASP
1	E	387	MET
1	F	22	SER
1	F	26	LYS
1	F	54	TRP
1	F	66	LYS
1	F	96	CYS
1	F	143	ARG
1	F	144	CYS
1	F	167	LYS
1	F	191	ASN
1	F	221	ASP
1	F	237	LEU
1	F	257	LEU
1	F	308	LEU
1	F	353	LEU
1	F	356	SER
1	F	364	LEU
1	F	382	GLN
1	F	383	SER
1	G	38	ASN
1	G	54	TRP
1	G	96	CYS
1	G	143	ARG
1	G	185	TYR
1	G	237	LEU
1	G	257	LEU
1	G	285	ASN
1	G	308	LEU
1	G	309	ARG
1	G	336	GLU
1	G	337	SER
1	G	353	LEU

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Mol	Chain	Res	Type
1	G	358	ARG
1	G	387	MET
1	H	22	SER
1	H	26	LYS
1	H	54	TRP
1	H	66	LYS
1	H	143	ARG
1	H	191	ASN
1	H	192	GLU
1	H	257	LEU
1	H	308	LEU
1	H	310	LEU
1	H	313	LEU
1	H	353	LEU
1	H	364	LEU
1	H	382	GLN
1	I	38	ASN
1	I	54	TRP
1	I	110	HIS
1	I	143	ARG
1	I	144	CYS
1	I	149	LYS
1	I	191	ASN
1	I	200	GLU
1	I	237	LEU
1	I	257	LEU
1	I	308	LEU
1	I	333	THR
1	I	337	SER
1	I	342	ASP
1	I	353	LEU
1	I	364	LEU
1	I	387	MET
1	J	22	SER
1	J	26	LYS
1	J	43	SER
1	J	54	TRP
1	J	66	LYS
1	J	97	TYR
1	J	134	ASP
1	J	143	ARG
1	J	191	ASN

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Mol	Chain	Res	Type
1	J	232	ASN
1	J	257	LEU
1	J	308	LEU
1	J	313	LEU
1	J	333	THR
1	J	353	LEU
1	J	364	LEU
1	J	382	GLN
1	K	38	ASN
1	K	66	LYS
1	K	134	ASP
1	K	143	ARG
1	K	149	LYS
1	K	151	VAL
1	K	191	ASN
1	K	200	GLU
1	K	257	LEU
1	K	285	ASN
1	K	308	LEU
1	K	342	ASP
1	K	346	ASP
1	K	353	LEU
1	K	364	LEU
1	K	383	SER
1	K	387	MET
1	L	10	VAL
1	L	22	SER
1	L	66	LYS
1	L	70	THR
1	L	132	PHE
1	L	143	ARG
1	L	212	LEU
1	L	232	ASN
1	L	237	LEU
1	L	242	GLU
1	L	257	LEU
1	L	305	SER
1	L	308	LEU
1	L	337	SER
1	L	346	ASP
1	L	353	LEU
1	L	358	ARG

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Mol	Chain	Res	Type
1	L	364	LEU
1	M	36	LYS
1	M	38	ASN
1	M	54	TRP
1	M	143	ARG
1	M	167	LYS
1	M	191	ASN
1	M	200	GLU
1	M	237	LEU
1	M	257	LEU
1	M	285	ASN
1	M	287	ARG
1	M	308	LEU
1	M	333	THR
1	M	353	LEU
1	M	364	LEU
1	M	382	GLN
1	N	22	SER
1	N	26	LYS
1	N	54	TRP
1	N	143	ARG
1	N	167	LYS
1	N	170	SER
1	N	191	ASN
1	N	221	ASP
1	N	237	LEU
1	N	257	LEU
1	N	263	ARG
1	N	276	LYS
1	N	308	LEU
1	N	313	LEU
1	N	352	ARG
1	N	353	LEU
1	N	364	LEU
1	N	382	GLN
1	N	386	ASP
1	O	38	ASN
1	O	54	TRP
1	O	74	ASN
1	O	134	ASP
1	O	143	ARG
1	O	200	GLU

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Mol	Chain	Res	Type
1	O	257	LEU
1	O	308	LEU
1	O	313	LEU
1	O	353	LEU
1	O	364	LEU
1	P	22	SER
1	P	103	LYS
1	P	110	HIS
1	P	144	CYS
1	P	147	SER
1	P	191	ASN
1	P	237	LEU
1	P	242	GLU
1	P	257	LEU
1	P	308	LEU
1	P	337	SER
1	P	353	LEU
1	P	364	LEU
1	Q	43	SER
1	Q	54	TRP
1	Q	58	THR
1	Q	68	ILE
1	Q	143	ARG
1	Q	144	CYS
1	Q	151	VAL
1	Q	200	GLU
1	Q	237	LEU
1	Q	257	LEU
1	Q	294	CYS
1	Q	308	LEU
1	Q	313	LEU
1	Q	341	THR
1	Q	342	ASP
1	Q	353	LEU
1	Q	364	LEU
1	Q	383	SER
1	Q	385	ASP
1	R	13	ARG
1	R	22	SER
1	R	26	LYS
1	R	54	TRP
1	R	66	LYS

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Mol	Chain	Res	Type
1	R	96	CYS
1	R	103	LYS
1	R	143	ARG
1	R	144	CYS
1	R	221	ASP
1	R	257	LEU
1	R	308	LEU
1	R	313	LEU
1	R	346	ASP
1	R	353	LEU
1	R	364	LEU
1	R	382	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (75) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	38	ASN
1	A	60	ASN
1	A	195	GLN
1	A	284	HIS
1	A	285	ASN
1	A	382	GLN
1	B	284	HIS
1	B	285	ASN
1	C	285	ASN
1	C	382	GLN
1	D	195	GLN
1	D	232	ASN
1	D	284	HIS
1	D	285	ASN
1	D	382	GLN
1	E	38	ASN
1	E	195	GLN
1	E	284	HIS
1	E	382	GLN
1	F	191	ASN
1	F	195	GLN
1	F	197	GLN
1	F	285	ASN
1	G	284	HIS
1	G	285	ASN
1	H	60	ASN

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Mol	Chain	Res	Type
1	H	110	HIS
1	H	195	GLN
1	H	284	HIS
1	H	285	ASN
1	I	38	ASN
1	I	69	GLN
1	I	110	HIS
1	I	195	GLN
1	I	285	ASN
1	J	110	HIS
1	J	125	ASN
1	J	191	ASN
1	J	195	GLN
1	J	280	HIS
1	J	284	HIS
1	J	285	ASN
1	K	38	ASN
1	K	191	ASN
1	K	195	GLN
1	K	285	ASN
1	K	382	GLN
1	L	60	ASN
1	L	195	GLN
1	L	241	ASN
1	L	285	ASN
1	M	38	ASN
1	M	195	GLN
1	M	285	ASN
1	M	307	HIS
1	N	16	HIS
1	N	191	ASN
1	N	285	ASN
1	O	38	ASN
1	O	285	ASN
1	O	382	GLN
1	P	195	GLN
1	P	280	HIS
1	P	285	ASN
1	P	369	ASN
1	Q	77	ASN
1	Q	124	HIS
1	Q	195	GLN

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Mol	Chain	Res	Type
1	Q	285	ASN
1	Q	369	ASN
1	R	69	GLN
1	R	195	GLN
1	R	280	HIS
1	R	285	ASN
1	R	382	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains 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 72 ligands modelled in this entry, 18 are monoatomic - leaving 54 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	$\# Z  > 2$
2	NMG	A	501	-	7,7,7	0.69	0	8,8,8	1.70	1 (12%)
3	ADP	A	601	4	29,29,29	1.07	2 (6%)	45,45,45	1.87	9 (20%)
5	NO3	A	801	4	3,3,3	3.23	3 (100%)	3,3,3	0.09	0
2	NMG	B	502	-	7,7,7	0.72	0	8,8,8	2.28	1 (12%)
3	ADP	B	602	4	29,29,29	1.11	2 (6%)	45,45,45	1.78	6 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	NO3	B	802	4	3,3,3	3.36	3 (100%)	3,3,3	0.10	0
2	NMG	C	503	-	7,7,7	0.72	0	8,8,8	1.49	1 (12%)
3	ADP	C	603	4	29,29,29	1.08	2 (6%)	45,45,45	1.78	8 (17%)
5	NO3	C	803	4	3,3,3	3.39	3 (100%)	3,3,3	0.26	0
2	NMG	D	504	-	7,7,7	0.75	0	8,8,8	1.63	1 (12%)
3	ADP	D	604	4	29,29,29	1.06	2 (6%)	45,45,45	1.75	6 (13%)
5	NO3	D	804	4	3,3,3	3.21	3 (100%)	3,3,3	0.15	0
2	NMG	E	505	-	7,7,7	0.72	0	8,8,8	1.62	1 (12%)
3	ADP	E	605	4	29,29,29	1.17	2 (6%)	45,45,45	1.94	8 (17%)
5	NO3	E	805	4	3,3,3	3.26	3 (100%)	3,3,3	0.21	0
2	NMG	F	506	-	7,7,7	0.70	0	8,8,8	1.89	2 (25%)
3	ADP	F	606	4	29,29,29	1.15	2 (6%)	45,45,45	2.02	12 (26%)
5	NO3	F	806	4	3,3,3	3.38	3 (100%)	3,3,3	0.17	0
2	NMG	G	507	-	7,7,7	0.74	0	8,8,8	1.38	1 (12%)
3	ADP	G	607	4	29,29,29	1.14	2 (6%)	45,45,45	1.89	7 (15%)
5	NO3	G	807	4	3,3,3	3.16	3 (100%)	3,3,3	0.14	0
2	NMG	H	508	-	7,7,7	0.78	0	8,8,8	1.48	1 (12%)
3	ADP	H	608	4	29,29,29	1.26	3 (10%)	45,45,45	1.59	7 (15%)
5	NO3	H	808	4	3,3,3	3.31	3 (100%)	3,3,3	0.26	0
2	NMG	I	509	-	7,7,7	0.78	0	8,8,8	1.94	1 (12%)
3	ADP	I	609	4	29,29,29	1.15	2 (6%)	45,45,45	1.85	8 (17%)
5	NO3	I	809	4	3,3,3	3.21	3 (100%)	3,3,3	0.11	0
2	NMG	J	510	-	7,7,7	0.71	0	8,8,8	1.77	1 (12%)
3	ADP	J	610	4	29,29,29	1.27	3 (10%)	45,45,45	1.85	10 (22%)
5	NO3	J	810	4	3,3,3	3.19	3 (100%)	3,3,3	0.20	0
2	NMG	K	511	-	7,7,7	0.72	0	8,8,8	1.68	1 (12%)
3	ADP	K	611	4	29,29,29	1.30	5 (17%)	45,45,45	1.74	9 (20%)
5	NO3	K	811	4	3,3,3	3.22	3 (100%)	3,3,3	0.15	0
2	NMG	L	512	-	7,7,7	0.74	0	8,8,8	1.62	1 (12%)
3	ADP	L	612	4	29,29,29	1.19	2 (6%)	45,45,45	1.69	7 (15%)
5	NO3	L	812	4	3,3,3	3.31	3 (100%)	3,3,3	0.10	0
2	NMG	M	513	-	7,7,7	0.69	0	8,8,8	1.60	1 (12%)
3	ADP	M	613	4	29,29,29	1.17	2 (6%)	45,45,45	1.97	9 (20%)
5	NO3	M	813	4	3,3,3	3.23	3 (100%)	3,3,3	0.12	0
2	NMG	N	514	-	7,7,7	0.74	0	8,8,8	1.50	1 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	ADP	N	614	4	29,29,29	1.18	3 (10%)	45,45,45	1.79	7 (15%)
5	NO3	N	814	4	3,3,3	3.25	3 (100%)	3,3,3	0.20	0
2	NMG	O	515	-	7,7,7	0.60	0	8,8,8	1.87	2 (25%)
3	ADP	O	615	4	29,29,29	1.19	2 (6%)	45,45,45	2.00	10 (22%)
5	NO3	O	815	4	3,3,3	3.28	3 (100%)	3,3,3	0.19	0
2	NMG	P	516	-	7,7,7	0.73	0	8,8,8	2.07	1 (12%)
3	ADP	P	616	4	29,29,29	1.12	2 (6%)	45,45,45	1.96	10 (22%)
5	NO3	P	816	-	3,3,3	3.34	3 (100%)	3,3,3	0.28	0
2	NMG	Q	517	-	7,7,7	0.78	0	8,8,8	1.34	1 (12%)
3	ADP	Q	617	4	29,29,29	1.12	2 (6%)	45,45,45	1.72	8 (17%)
5	NO3	Q	817	4	3,3,3	3.25	3 (100%)	3,3,3	0.12	0
2	NMG	R	518	-	7,7,7	0.84	0	8,8,8	1.98	1 (12%)
3	ADP	R	618	4	29,29,29	1.20	4 (13%)	45,45,45	1.84	9 (20%)
5	NO3	R	818	4	3,3,3	3.35	3 (100%)	3,3,3	0.10	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
2	NMG	A	501	-	-	0/5/5/5	0/0/0/0
3	ADP	A	601	4	-	0/16/32/32	0/1/3/3
5	NO3	A	801	4	-	0/0/0/0	0/0/0/0
2	NMG	B	502	-	-	0/5/5/5	0/0/0/0
3	ADP	B	602	4	-	0/16/32/32	0/1/3/3
5	NO3	B	802	4	-	0/0/0/0	0/0/0/0
2	NMG	C	503	-	-	0/5/5/5	0/0/0/0
3	ADP	C	603	4	-	0/16/32/32	0/1/3/3
5	NO3	C	803	4	-	0/0/0/0	0/0/0/0
2	NMG	D	504	-	-	0/5/5/5	0/0/0/0
3	ADP	D	604	4	-	0/16/32/32	0/1/3/3
5	NO3	D	804	4	-	0/0/0/0	0/0/0/0
2	NMG	E	505	-	-	0/5/5/5	0/0/0/0
3	ADP	E	605	4	-	0/16/32/32	0/1/3/3
5	NO3	E	805	4	-	0/0/0/0	0/0/0/0
2	NMG	F	506	-	-	0/5/5/5	0/0/0/0
3	ADP	F	606	4	-	0/16/32/32	0/1/3/3
5	NO3	F	806	4	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NMG	G	507	-	-	0/5/5/5	0/0/0/0
3	ADP	G	607	4	-	0/16/32/32	0/1/3/3
5	NO3	G	807	4	-	0/0/0/0	0/0/0/0
2	NMG	H	508	-	-	0/5/5/5	0/0/0/0
3	ADP	H	608	4	-	0/16/32/32	0/1/3/3
5	NO3	H	808	4	-	0/0/0/0	0/0/0/0
2	NMG	I	509	-	-	0/5/5/5	0/0/0/0
3	ADP	I	609	4	-	0/16/32/32	0/1/3/3
5	NO3	I	809	4	-	0/0/0/0	0/0/0/0
2	NMG	J	510	-	-	0/5/5/5	0/0/0/0
3	ADP	J	610	4	-	0/16/32/32	0/1/3/3
5	NO3	J	810	4	-	0/0/0/0	0/0/0/0
2	NMG	K	511	-	-	0/5/5/5	0/0/0/0
3	ADP	K	611	4	-	0/16/32/32	0/1/3/3
5	NO3	K	811	4	-	0/0/0/0	0/0/0/0
2	NMG	L	512	-	-	0/5/5/5	0/0/0/0
3	ADP	L	612	4	-	0/16/32/32	0/1/3/3
5	NO3	L	812	4	-	0/0/0/0	0/0/0/0
2	NMG	M	513	-	-	0/5/5/5	0/0/0/0
3	ADP	M	613	4	-	0/16/32/32	0/1/3/3
5	NO3	M	813	4	-	0/0/0/0	0/0/0/0
2	NMG	N	514	-	-	0/5/5/5	0/0/0/0
3	ADP	N	614	4	-	0/16/32/32	0/1/3/3
5	NO3	N	814	4	-	0/0/0/0	0/0/0/0
2	NMG	O	515	-	-	0/5/5/5	0/0/0/0
3	ADP	O	615	4	-	0/16/32/32	0/1/3/3
5	NO3	O	815	4	-	0/0/0/0	0/0/0/0
2	NMG	P	516	-	-	0/5/5/5	0/0/0/0
3	ADP	P	616	4	-	0/16/32/32	0/1/3/3
5	NO3	P	816	-	-	0/0/0/0	0/0/0/0
2	NMG	Q	517	-	-	0/5/5/5	0/0/0/0
3	ADP	Q	617	4	-	0/16/32/32	0/1/3/3
5	NO3	Q	817	4	-	0/0/0/0	0/0/0/0
2	NMG	R	518	-	-	0/5/5/5	0/0/0/0
3	ADP	R	618	4	-	0/16/32/32	0/1/3/3
5	NO3	R	818	4	-	0/0/0/0	0/0/0/0

All (98) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	803	NO3	O1-N	4.05	1.41	1.24
5	F	806	NO3	O1-N	4.03	1.41	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	802	NO3	O1-N	4.03	1.41	1.24
5	I	809	NO3	O1-N	3.97	1.41	1.24
5	R	818	NO3	O1-N	3.96	1.41	1.24
5	L	812	NO3	O1-N	3.95	1.41	1.24
5	O	815	NO3	O1-N	3.88	1.40	1.24
3	J	610	ADP	C4-N9	-3.87	1.32	1.37
5	Q	817	NO3	O1-N	3.86	1.40	1.24
5	H	808	NO3	O1-N	3.86	1.40	1.24
5	A	801	NO3	O1-N	3.84	1.40	1.24
5	P	816	NO3	O1-N	3.83	1.40	1.24
5	M	813	NO3	O1-N	3.83	1.40	1.24
5	N	814	NO3	O1-N	3.80	1.40	1.24
5	G	807	NO3	O1-N	3.79	1.40	1.24
5	K	811	NO3	O1-N	3.79	1.40	1.24
5	E	805	NO3	O1-N	3.78	1.40	1.24
5	D	804	NO3	O1-N	3.77	1.40	1.24
5	J	810	NO3	O1-N	3.74	1.40	1.24
3	H	608	ADP	C4-N9	-3.69	1.32	1.37
3	L	612	ADP	C4-N9	-3.61	1.32	1.37
3	F	606	ADP	C4-N9	-3.51	1.32	1.37
3	M	613	ADP	C4-N9	-3.50	1.32	1.37
3	O	615	ADP	C4-N9	-3.49	1.32	1.37
3	K	611	ADP	C4-N9	-3.49	1.32	1.37
3	E	605	ADP	C5-C4	3.26	1.47	1.40
3	Q	617	ADP	C5-C4	3.24	1.47	1.40
3	R	618	ADP	C5-C4	3.19	1.47	1.40
3	R	618	ADP	C4-N9	-3.17	1.33	1.37
3	I	609	ADP	C4-N9	-3.16	1.33	1.37
3	P	616	ADP	C4-N9	-3.14	1.33	1.37
3	N	614	ADP	C5-C4	3.13	1.47	1.40
5	P	816	NO3	O2-N	3.12	1.41	1.25
5	C	803	NO3	O3-N	3.11	1.41	1.25
3	C	603	ADP	C5-C4	3.10	1.47	1.40
5	F	806	NO3	O3-N	3.07	1.41	1.25
3	C	603	ADP	C4-N9	-3.07	1.33	1.37
3	D	604	ADP	C5-C4	3.06	1.47	1.40
5	H	808	NO3	O2-N	3.05	1.41	1.25
3	A	601	ADP	C5-C4	3.04	1.47	1.40
5	E	805	NO3	O3-N	3.03	1.41	1.25
3	B	602	ADP	C5-C4	3.02	1.47	1.40
5	P	816	NO3	O3-N	3.01	1.41	1.25
3	O	615	ADP	C5-C4	3.01	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	R	818	NO3	O3-N	3.00	1.41	1.25
5	O	815	NO3	O3-N	3.00	1.41	1.25
5	R	818	NO3	O2-N	2.99	1.41	1.25
5	L	812	NO3	O2-N	2.99	1.41	1.25
3	G	607	ADP	C4-N9	-2.98	1.33	1.37
3	P	616	ADP	C5-C4	2.97	1.47	1.40
5	B	802	NO3	O2-N	2.97	1.41	1.25
5	K	811	NO3	O3-N	2.96	1.41	1.25
5	D	804	NO3	O3-N	2.96	1.41	1.25
5	A	801	NO3	O2-N	2.96	1.41	1.25
3	F	606	ADP	C5-C4	2.96	1.47	1.40
5	B	802	NO3	O3-N	2.95	1.41	1.25
5	Q	817	NO3	O3-N	2.95	1.41	1.25
5	N	814	NO3	O3-N	2.95	1.41	1.25
3	H	608	ADP	C5-C4	2.94	1.47	1.40
3	N	614	ADP	C4-N9	-2.94	1.33	1.37
5	F	806	NO3	O2-N	2.94	1.40	1.25
5	J	810	NO3	O3-N	2.93	1.40	1.25
5	H	808	NO3	O3-N	2.93	1.40	1.25
3	Q	617	ADP	C4-N9	-2.92	1.33	1.37
5	N	814	NO3	O2-N	2.92	1.40	1.25
3	K	611	ADP	C5-C4	2.92	1.47	1.40
5	C	803	NO3	O2-N	2.91	1.40	1.25
5	L	812	NO3	O3-N	2.91	1.40	1.25
5	M	813	NO3	O3-N	2.90	1.40	1.25
3	J	610	ADP	C5-C4	2.89	1.47	1.40
5	E	805	NO3	O2-N	2.89	1.40	1.25
3	E	605	ADP	C4-N9	-2.87	1.33	1.37
5	M	813	NO3	O2-N	2.87	1.40	1.25
3	I	609	ADP	C5-C4	2.85	1.46	1.40
5	O	815	NO3	O2-N	2.85	1.40	1.25
5	G	807	NO3	O2-N	2.85	1.40	1.25
5	Q	817	NO3	O2-N	2.85	1.40	1.25
3	L	612	ADP	C5-C4	2.84	1.46	1.40
3	M	613	ADP	C5-C4	2.84	1.46	1.40
3	G	607	ADP	C5-C4	2.83	1.46	1.40
3	B	602	ADP	C4-N9	-2.82	1.33	1.37
5	J	810	NO3	O2-N	2.81	1.40	1.25
5	K	811	NO3	O2-N	2.81	1.40	1.25
5	D	804	NO3	O2-N	2.80	1.40	1.25
5	A	801	NO3	O3-N	2.78	1.40	1.25
5	I	809	NO3	O2-N	2.76	1.39	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	I	809	NO3	O3-N	2.74	1.39	1.25
5	G	807	NO3	O3-N	2.74	1.39	1.25
3	A	601	ADP	C4-N9	-2.61	1.33	1.37
3	D	604	ADP	C4-N9	-2.43	1.34	1.37
3	J	610	ADP	PA-O3A	2.21	1.63	1.59
3	H	608	ADP	PA-O3A	2.18	1.63	1.59
3	K	611	ADP	C2'-C1'	-2.14	1.50	1.53
3	R	618	ADP	PA-O3A	2.13	1.63	1.59
3	K	611	ADP	PA-O3A	2.09	1.63	1.59
3	R	618	ADP	PB-O3A	2.09	1.63	1.60
3	K	611	ADP	PB-O3A	2.06	1.63	1.60
3	N	614	ADP	PB-O3A	2.04	1.63	1.60

All (170) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	606	ADP	N3-C2-N1	-7.77	122.21	128.71
3	O	615	ADP	N3-C2-N1	-7.47	122.47	128.71
3	G	607	ADP	N3-C2-N1	-7.31	122.60	128.71
3	M	613	ADP	N3-C2-N1	-7.27	122.63	128.71
3	P	616	ADP	N3-C2-N1	-7.21	122.68	128.71
3	A	601	ADP	N3-C2-N1	-7.19	122.70	128.71
3	R	618	ADP	N3-C2-N1	-7.16	122.72	128.71
3	J	610	ADP	N3-C2-N1	-7.12	122.75	128.71
3	C	603	ADP	N3-C2-N1	-7.07	122.80	128.71
3	N	614	ADP	N3-C2-N1	-7.01	122.84	128.71
3	I	609	ADP	N3-C2-N1	-6.74	123.07	128.71
3	D	604	ADP	N3-C2-N1	-6.63	123.17	128.71
3	Q	617	ADP	N3-C2-N1	-6.40	123.36	128.71
3	L	612	ADP	N3-C2-N1	-6.23	123.50	128.71
3	K	611	ADP	N3-C2-N1	-6.14	123.57	128.71
3	B	602	ADP	N3-C2-N1	-6.13	123.58	128.71
3	E	605	ADP	O4'-C1'-N9	6.12	114.13	108.44
3	H	608	ADP	N3-C2-N1	-6.06	123.64	128.71
3	E	605	ADP	N3-C2-N1	-5.86	123.81	128.71
2	B	502	NMG	CD-NE-CZ	5.76	129.66	121.34
2	P	516	NMG	CD-NE-CZ	5.42	129.17	121.34
3	E	605	ADP	N3-C4-N9	5.39	135.16	125.43
3	D	604	ADP	N3-C4-N9	5.35	135.09	125.43
3	H	608	ADP	N3-C4-N9	5.28	134.97	125.43
3	G	607	ADP	N3-C4-N9	5.20	134.83	125.43
3	B	602	ADP	N3-C4-N9	5.15	134.72	125.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	R	518	NMG	CD-NE-CZ	5.13	128.75	121.34
3	Q	617	ADP	N3-C4-N9	5.09	134.62	125.43
3	O	615	ADP	N3-C4-N9	4.98	134.43	125.43
3	M	613	ADP	O4'-C1'-N9	4.97	113.06	108.44
3	P	616	ADP	N3-C4-N9	4.95	134.36	125.43
3	C	603	ADP	N3-C4-N9	4.93	134.33	125.43
2	I	509	NMG	CD-NE-CZ	4.93	128.46	121.34
3	I	609	ADP	N3-C4-N9	4.92	134.32	125.43
3	A	601	ADP	N3-C4-N9	4.88	134.24	125.43
3	N	614	ADP	N3-C4-N9	4.83	134.15	125.43
2	F	506	NMG	CD-NE-CZ	4.62	128.01	121.34
2	O	515	NMG	CD-NE-CZ	4.57	127.94	121.34
3	R	618	ADP	N3-C4-N9	4.52	133.59	125.43
3	F	606	ADP	N3-C4-N9	4.48	133.52	125.43
3	K	611	ADP	N3-C4-N9	4.43	133.43	125.43
3	L	612	ADP	N3-C4-N9	4.40	133.38	125.43
2	J	510	NMG	CD-NE-CZ	4.40	127.69	121.34
3	F	606	ADP	C8-N9-C4	4.33	110.21	106.90
2	A	501	NMG	CD-NE-CZ	4.29	127.54	121.34
3	J	610	ADP	N3-C4-N9	4.27	133.14	125.43
3	M	613	ADP	N3-C4-N9	4.27	133.14	125.43
3	O	615	ADP	O4'-C1'-N9	-4.12	104.61	108.44
2	D	504	NMG	CD-NE-CZ	4.12	127.29	121.34
2	K	511	NMG	CD-NE-CZ	4.08	127.23	121.34
2	L	512	NMG	CD-NE-CZ	4.05	127.20	121.34
2	E	505	NMG	CD-NE-CZ	3.97	127.07	121.34
2	N	514	NMG	CD-NE-CZ	3.78	126.80	121.34
3	O	615	ADP	C8-N9-C4	3.78	109.78	106.90
3	A	601	ADP	O4'-C1'-N9	3.77	111.95	108.44
2	M	513	NMG	CD-NE-CZ	3.76	126.77	121.34
3	K	611	ADP	C4-C5-N7	-3.75	106.31	109.52
3	B	602	ADP	C4-C5-N7	-3.63	106.41	109.52
3	G	607	ADP	C8-N9-C4	3.59	109.64	106.90
3	N	614	ADP	C4-C5-N7	-3.57	106.47	109.52
3	I	609	ADP	C8-N9-C4	3.57	109.62	106.90
2	C	503	NMG	CD-NE-CZ	3.55	126.47	121.34
2	H	508	NMG	CD-NE-CZ	3.53	126.44	121.34
3	J	610	ADP	C8-N9-C4	3.50	109.57	106.90
3	B	602	ADP	C8-N9-C4	3.47	109.55	106.90
3	M	613	ADP	C4-C5-N7	-3.44	106.57	109.52
3	R	618	ADP	C4-C5-N7	-3.36	106.65	109.52
3	E	605	ADP	C5-C4-N3	-3.35	118.41	125.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	605	ADP	C4-C5-N7	-3.31	106.68	109.52
3	L	612	ADP	C4-C5-N7	-3.22	106.76	109.52
3	P	616	ADP	PA-O3A-PB	3.22	141.12	131.68
3	K	611	ADP	C8-N9-C4	3.18	109.32	106.90
3	D	604	ADP	C8-N9-C4	3.16	109.31	106.90
3	Q	617	ADP	C4-C5-N7	-3.16	106.82	109.52
3	M	613	ADP	C1'-N9-C4	-3.13	121.23	126.64
3	F	606	ADP	O4'-C4'-C5'	-3.11	98.25	109.36
2	Q	517	NMG	CD-NE-CZ	3.10	125.82	121.34
2	G	507	NMG	CD-NE-CZ	3.06	125.76	121.34
3	P	616	ADP	C4-C5-N7	-3.06	106.90	109.52
3	R	618	ADP	C8-N9-C4	3.01	109.20	106.90
3	Q	617	ADP	C5-C4-N3	-3.01	119.15	125.70
3	B	602	ADP	C5-C4-N3	-3.01	119.15	125.70
3	D	604	ADP	C5-C4-N3	-2.95	119.28	125.70
3	H	608	ADP	C8-N9-C4	2.93	109.14	106.90
3	J	610	ADP	C1'-N9-C4	-2.93	121.58	126.64
3	N	614	ADP	C8-N9-C4	2.91	109.12	106.90
3	H	608	ADP	C5-C4-N3	-2.90	119.39	125.70
3	P	616	ADP	C5-C4-N3	-2.88	119.42	125.70
3	G	607	ADP	C4-C5-N7	-2.88	107.06	109.52
3	F	606	ADP	C4-C5-N7	-2.87	107.06	109.52
3	L	612	ADP	C8-N9-C4	2.86	109.08	106.90
3	D	604	ADP	C4-C5-N7	-2.86	107.07	109.52
3	G	607	ADP	C5-C4-N3	-2.83	119.53	125.70
3	N	614	ADP	C5-C4-N3	-2.83	119.54	125.70
3	A	601	ADP	C8-N9-C4	2.82	109.05	106.90
3	I	609	ADP	C4-C5-N7	-2.81	107.11	109.52
3	G	607	ADP	O4'-C1'-N9	-2.79	105.85	108.44
3	A	601	ADP	C4-C5-N7	-2.78	107.14	109.52
3	P	616	ADP	C8-N9-C4	2.78	109.02	106.90
3	M	613	ADP	C8-N9-C4	2.77	109.02	106.90
3	O	615	ADP	C4-C5-N7	-2.72	107.19	109.52
3	F	606	ADP	C1'-N9-C4	-2.72	121.94	126.64
3	J	610	ADP	O4'-C1'-N9	2.68	110.94	108.44
3	J	610	ADP	C4-C5-N7	-2.67	107.23	109.52
3	C	603	ADP	C5-C4-N3	-2.67	119.89	125.70
3	I	609	ADP	C5-C4-N3	-2.67	119.89	125.70
3	A	601	ADP	C5-C4-N3	-2.65	119.93	125.70
3	O	615	ADP	C5-C4-N3	-2.64	119.96	125.70
3	C	603	ADP	C8-N9-C4	2.62	108.90	106.90
3	K	611	ADP	C5-C4-N3	-2.61	120.01	125.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	606	ADP	O4'-C1'-N9	2.61	110.87	108.44
3	F	606	ADP	PA-O3A-PB	-2.56	124.18	131.68
3	I	609	ADP	C1'-N9-C4	-2.56	122.22	126.64
3	R	618	ADP	C1'-N9-C4	-2.55	122.23	126.64
3	R	618	ADP	C5-C4-N3	-2.53	120.18	125.70
3	G	607	ADP	C2-N3-C4	2.53	121.22	114.01
3	E	605	ADP	C2-N3-C4	2.53	121.22	114.01
3	M	613	ADP	C5-C4-N3	-2.52	120.20	125.70
3	C	603	ADP	C4-C5-N7	-2.52	107.36	109.52
3	F	606	ADP	C2-N1-C6	2.51	123.31	118.77
3	B	602	ADP	C2-N3-C4	2.50	121.14	114.01
3	A	601	ADP	O3B-PB-O2B	2.48	117.27	107.61
3	P	616	ADP	C2-N3-C4	2.48	121.06	114.01
3	L	612	ADP	C5-C4-N3	-2.45	120.37	125.70
3	D	604	ADP	C2-N3-C4	2.44	120.96	114.01
3	R	618	ADP	O4'-C1'-N9	2.44	110.70	108.44
3	O	615	ADP	C2-N3-C4	2.39	120.82	114.01
3	K	611	ADP	O4'-C1'-N9	2.39	110.66	108.44
3	M	613	ADP	C2-N3-C4	2.39	120.80	114.01
3	A	601	ADP	C2-N3-C4	2.35	120.71	114.01
3	I	609	ADP	C2-N3-C4	2.35	120.70	114.01
3	Q	617	ADP	C2-N3-C4	2.35	120.70	114.01
3	K	611	ADP	C1'-N9-C4	-2.34	122.59	126.64
3	P	616	ADP	C2'-C1'-N9	-2.33	107.28	113.27
3	N	614	ADP	C2-N3-C4	2.33	120.64	114.01
3	P	616	ADP	C3'-C2'-C1'	2.33	104.55	100.91
3	R	618	ADP	C2-N3-C4	2.32	120.62	114.01
3	K	611	ADP	O3'-C3'-C4'	-2.30	104.29	111.08
3	C	603	ADP	C2-N3-C4	2.30	120.55	114.01
3	Q	617	ADP	O4'-C1'-N9	-2.29	106.31	108.44
3	N	614	ADP	C2-N1-C6	2.28	122.88	118.77
3	J	610	ADP	O4'-C4'-C5'	-2.27	101.25	109.36
3	L	612	ADP	C1'-N9-C4	-2.24	122.76	126.64
3	P	616	ADP	O3A-PA-O5'	2.24	113.40	103.41
3	J	610	ADP	C5-C4-N3	-2.22	120.87	125.70
3	Q	617	ADP	C8-N9-C4	2.21	108.59	106.90
3	J	610	ADP	C2-N1-C6	2.21	122.76	118.77
3	H	608	ADP	C2-N3-C4	2.20	120.28	114.01
3	R	618	ADP	C2-N1-C6	2.20	122.74	118.77
3	F	606	ADP	C2-N3-C4	2.20	120.27	114.01
3	F	606	ADP	O5'-C5'-C4'	2.19	116.99	108.94
3	E	605	ADP	O3B-PB-O2B	2.18	116.09	107.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	605	ADP	C8-N9-C4	2.17	108.56	106.90
3	O	615	ADP	C2-N1-C6	2.17	122.69	118.77
3	K	611	ADP	C2-N3-C4	2.17	120.19	114.01
3	F	606	ADP	C5-C4-N3	-2.17	120.98	125.70
3	J	610	ADP	C2-N3-C4	2.17	120.18	114.01
3	C	603	ADP	O3B-PB-O2B	2.15	116.00	107.61
3	M	613	ADP	C2-N1-C6	2.13	122.62	118.77
3	L	612	ADP	C2-N3-C4	2.11	120.02	114.01
3	O	615	ADP	O5'-PA-O1A	-2.09	101.20	109.37
3	C	603	ADP	C2-N1-C6	2.07	122.51	118.77
3	A	601	ADP	C2-N1-C6	2.06	122.49	118.77
2	O	515	NMG	O1-CG-CD	2.06	120.45	112.98
3	H	608	ADP	C4-C5-N7	-2.05	107.77	109.52
2	F	506	NMG	CG-CD-NE	-2.05	107.93	112.83
3	Q	617	ADP	C3'-C2'-C1'	2.04	104.10	100.91
3	H	608	ADP	C2'-C3'-C4'	2.01	106.67	102.65
3	I	609	ADP	PA-O3A-PB	-2.01	125.80	131.68
3	O	615	ADP	O3A-PA-O5'	2.00	112.36	103.41

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 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(Å²)	Q<0.9
1	A	367/390 (94%)	2.16	168 (45%)	1	1	18, 30, 47, 54	0
1	B	388/390 (99%)	1.87	144 (37%)	1	1	15, 25, 46, 58	0
1	C	367/390 (94%)	1.89	144 (39%)	1	1	17, 26, 40, 52	0
1	D	385/390 (98%)	2.01	158 (41%)	1	1	16, 27, 46, 59	0
1	E	367/390 (94%)	2.02	162 (44%)	1	1	18, 29, 45, 53	0
1	F	382/390 (97%)	1.73	124 (32%)	1	1	13, 24, 42, 55	0
1	G	367/390 (94%)	1.98	159 (43%)	1	1	16, 27, 42, 54	0
1	H	382/390 (97%)	1.77	132 (34%)	1	1	15, 23, 41, 55	0
1	I	367/390 (94%)	2.07	154 (41%)	1	1	17, 26, 41, 51	0
1	J	385/390 (98%)	1.84	139 (36%)	1	1	17, 25, 42, 61	0
1	K	367/390 (94%)	2.11	178 (48%)	1	0	17, 26, 42, 50	0
1	L	381/390 (97%)	2.23	193 (50%)	0	0	20, 31, 48, 59	0
1	M	367/390 (94%)	2.57	217 (59%)	0	0	17, 26, 41, 51	0
1	N	382/390 (97%)	2.65	223 (58%)	0	0	18, 27, 44, 52	0
1	O	367/390 (94%)	1.91	147 (40%)	1	1	16, 25, 40, 51	0
1	P	382/390 (97%)	1.93	140 (36%)	1	1	15, 24, 41, 50	0
1	Q	366/390 (93%)	2.54	211 (57%)	0	0	19, 30, 44, 53	0
1	R	381/390 (97%)	2.14	169 (44%)	1	1	15, 24, 40, 51	0
All	All	6750/7020 (96%)	2.08	2962 (43%)	1	1	13, 26, 44, 61	0

All (2962) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	M	282	LEU	12.3
1	M	281	GLY	12.3
1	B	381	GLY	11.9

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Mol	Chain	Res	Type	RSRZ
1	M	328	LEU	11.7
1	N	87	VAL	10.6
1	P	19	PRO	10.6
1	J	7	ASP	10.4
1	K	299	GLY	10.2
1	N	124	HIS	9.5
1	B	10	VAL	9.5
1	D	10	VAL	9.4
1	M	148	VAL	9.4
1	N	22	SER	9.3
1	J	8	TYR	9.3
1	L	328	LEU	9.2
1	G	278	CYS	9.1
1	Q	164	LEU	9.1
1	K	278	CYS	8.9
1	N	280	HIS	8.9
1	R	22	SER	8.7
1	M	187	LEU	8.6
1	N	19	PRO	8.5
1	N	10	VAL	8.4
1	M	228	ILE	8.2
1	N	99	GLU	8.1
1	F	10	VAL	8.0
1	Q	261	PHE	8.0
1	K	131	VAL	7.9
1	N	370	LEU	7.9
1	Q	152	CYS	7.8
1	I	187	LEU	7.7
1	P	15	GLY	7.7
1	O	176	LEU	7.6
1	J	286	ASP	7.6
1	L	353	LEU	7.6
1	Q	340	ALA	7.6
1	F	9	PHE	7.4
1	R	152	CYS	7.3
1	N	15	GLY	7.2
1	Q	61	GLY	7.2
1	D	278	CYS	7.1
1	Q	70	THR	7.1
1	B	5	ILE	7.1
1	D	356	SER	7.1
1	E	27	ALA	7.0

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Mol	Chain	Res	Type	RSRZ
1	J	6	GLN	7.0
1	N	274	LEU	7.0
1	C	151	VAL	7.0
1	N	9	PHE	7.0
1	L	136	TYR	6.9
1	R	168	VAL	6.9
1	M	165	VAL	6.9
1	N	288	LEU	6.9
1	D	385	ASP	6.8
1	M	169	VAL	6.8
1	G	24	LYS	6.7
1	N	278	CYS	6.7
1	P	378	LEU	6.7
1	I	364	LEU	6.7
1	F	96	CYS	6.7
1	Q	248	VAL	6.7
1	D	132	PHE	6.6
1	D	390	LYS	6.6
1	C	238	VAL	6.6
1	O	122	LEU	6.6
1	M	28	ALA	6.6
1	M	93	SER	6.6
1	L	313	LEU	6.6
1	N	33	ASP	6.6
1	R	160	ALA	6.5
1	F	12	ASN	6.5
1	P	20	TRP	6.5
1	K	380	ALA	6.5
1	Q	246	ILE	6.5
1	D	312	PHE	6.4
1	A	378	LEU	6.4
1	I	131	VAL	6.4
1	R	378	LEU	6.4
1	M	86	CYS	6.4
1	K	96	CYS	6.3
1	N	131	VAL	6.3
1	M	185	TYR	6.2
1	H	383	SER	6.2
1	J	9	PHE	6.2
1	Q	80	TYR	6.2
1	R	14	VAL	6.2
1	A	27	ALA	6.2

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Mol	Chain	Res	Type	RSRZ
1	N	279	GLY	6.2
1	M	152	CYS	6.2
1	A	151	VAL	6.1
1	A	25	PHE	6.1
1	H	328	LEU	6.1
1	O	136	TYR	6.1
1	M	329	GLY	6.1
1	I	373	ALA	6.1
1	J	129	GLY	6.1
1	A	367	GLY	6.0
1	A	133	GLU	6.0
1	Q	282	LEU	6.0
1	N	16	HIS	6.0
1	L	119	ALA	6.0
1	I	292	CYS	5.9
1	F	281	GLY	5.9
1	R	248	VAL	5.9
1	M	267	GLY	5.9
1	J	22	SER	5.9
1	Q	319	PHE	5.9
1	D	308	LEU	5.8
1	A	228	ILE	5.8
1	Q	136	TYR	5.8
1	N	310	LEU	5.8
1	Q	381	GLY	5.8
1	N	152	CYS	5.8
1	D	12	ASN	5.8
1	H	122	LEU	5.8
1	N	323	LEU	5.8
1	E	118	PRO	5.8
1	G	54	TRP	5.7
1	M	351	ALA	5.7
1	R	20	TRP	5.7
1	Q	40	VAL	5.7
1	N	291	ILE	5.7
1	P	136	TYR	5.7
1	R	176	LEU	5.7
1	I	61	GLY	5.6
1	H	22	SER	5.6
1	B	388	ILE	5.6
1	N	113	PRO	5.6
1	N	114	SER	5.6

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Mol	Chain	Res	Type	RSRZ
1	L	363	VAL	5.6
1	Q	99	GLU	5.6
1	A	54	TRP	5.6
1	M	40	VAL	5.6
1	F	313	LEU	5.6
1	P	16	HIS	5.5
1	O	25	PHE	5.5
1	A	92	TYR	5.5
1	K	184	TYR	5.5
1	Q	285	ASN	5.5
1	A	317	PRO	5.5
1	L	22	SER	5.5
1	P	361	VAL	5.5
1	L	386	ASP	5.4
1	E	85	GLY	5.4
1	H	286	ASP	5.4
1	L	175	GLY	5.4
1	P	18	LYS	5.4
1	L	171	ASP	5.4
1	L	25	PHE	5.4
1	N	175	GLY	5.3
1	B	312	PHE	5.3
1	A	309	ARG	5.3
1	G	219	ALA	5.3
1	B	6	GLN	5.3
1	N	29	ASP	5.3
1	N	268	LEU	5.3
1	C	311	ALA	5.3
1	L	360	LEU	5.3
1	C	385	ASP	5.3
1	Q	25	PHE	5.3
1	P	128	VAL	5.3
1	Q	67	CYS	5.3
1	R	13	ARG	5.3
1	Q	279	GLY	5.3
1	D	42	ALA	5.3
1	G	26	LYS	5.3
1	N	237	LEU	5.3
1	Q	45	LEU	5.3
1	K	81	GLY	5.2
1	N	232	ASN	5.2
1	M	387	MET	5.2

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Mol	Chain	Res	Type	RSRZ
1	R	122	LEU	5.2
1	Q	89	GLY	5.2
1	B	354	GLY	5.2
1	M	340	ALA	5.2
1	B	308	LEU	5.2
1	J	240	ILE	5.2
1	B	385	ASP	5.2
1	M	357	GLU	5.2
1	A	264	PHE	5.2
1	K	132	PHE	5.2
1	E	151	VAL	5.2
1	A	100	PHE	5.2
1	E	378	LEU	5.1
1	Q	225	GLY	5.1
1	M	271	VAL	5.1
1	P	122	LEU	5.1
1	N	88	PHE	5.1
1	A	176	LEU	5.1
1	M	45	LEU	5.1
1	D	388	ILE	5.1
1	R	17	SER	5.1
1	R	199	ILE	5.1
1	A	227	GLY	5.1
1	L	130	GLY	5.1
1	R	354	GLY	5.1
1	N	285	ASN	5.0
1	R	198	LEU	5.0
1	M	372	ILE	5.0
1	Q	142	ILE	5.0
1	I	35	SER	5.0
1	G	269	LEU	5.0
1	O	70	THR	5.0
1	R	280	HIS	5.0
1	E	264	PHE	5.0
1	M	323	LEU	5.0
1	M	368	VAL	5.0
1	I	28	ALA	5.0
1	K	174	GLY	5.0
1	P	280	HIS	5.0
1	A	58	THR	5.0
1	L	169	VAL	5.0
1	I	96	CYS	5.0

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Mol	Chain	Res	Type	RSRZ
1	N	26	LYS	5.0
1	N	132	PHE	5.0
1	A	229	TRP	4.9
1	N	351	ALA	4.9
1	Q	96	CYS	4.9
1	M	232	ASN	4.9
1	N	108	ILE	4.9
1	I	278	CYS	4.9
1	L	193	LYS	4.9
1	E	386	ASP	4.9
1	A	310	LEU	4.9
1	A	175	GLY	4.9
1	E	24	LYS	4.9
1	Q	286	ASP	4.9
1	Q	187	LEU	4.9
1	M	248	VAL	4.9
1	P	14	VAL	4.9
1	N	188	THR	4.9
1	L	345	TYR	4.8
1	R	21	GLU	4.8
1	N	313	LEU	4.8
1	A	255	GLY	4.8
1	F	284	HIS	4.8
1	Q	298	MET	4.8
1	K	171	ASP	4.8
1	Q	199	ILE	4.8
1	N	104	CYS	4.8
1	A	341	THR	4.8
1	K	239	TRP	4.8
1	N	387	MET	4.8
1	I	286	ASP	4.8
1	Q	278	CYS	4.8
1	Q	387	MET	4.8
1	M	180	LEU	4.8
1	R	238	VAL	4.8
1	E	341	THR	4.8
1	K	59	PRO	4.8
1	Q	124	HIS	4.8
1	C	165	VAL	4.8
1	D	184	TYR	4.8
1	R	128	VAL	4.8
1	E	354	GLY	4.7

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Mol	Chain	Res	Type	RSRZ
1	L	387	MET	4.7
1	H	385	ASP	4.7
1	I	333	THR	4.7
1	F	354	GLY	4.7
1	L	227	GLY	4.7
1	N	23	GLY	4.7
1	N	150	GLY	4.7
1	G	200	GLU	4.7
1	A	339	LEU	4.7
1	D	185	TYR	4.7
1	N	297	ASN	4.7
1	A	192	GLU	4.7
1	H	9	PHE	4.7
1	P	124	HIS	4.7
1	K	60	ASN	4.7
1	C	111	PHE	4.7
1	F	380	ALA	4.7
1	I	388	ILE	4.7
1	H	387	MET	4.7
1	N	122	LEU	4.6
1	C	148	VAL	4.6
1	B	291	ILE	4.6
1	H	388	ILE	4.6
1	E	229	TRP	4.6
1	L	286	ASP	4.6
1	E	192	GLU	4.6
1	Q	216	SER	4.6
1	N	101	PHE	4.6
1	E	360	LEU	4.6
1	K	122	LEU	4.6
1	Q	198	LEU	4.6
1	C	317	PRO	4.6
1	L	128	VAL	4.6
1	B	3	SER	4.6
1	D	22	SER	4.6
1	G	388	ILE	4.6
1	E	365	VAL	4.6
1	Q	135	LYS	4.6
1	N	64	PHE	4.6
1	H	85	GLY	4.6
1	B	96	CYS	4.6
1	E	164	LEU	4.6

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Mol	Chain	Res	Type	RSRZ
1	R	372	ILE	4.6
1	I	136	TYR	4.6
1	N	70	THR	4.6
1	Q	109	HIS	4.5
1	L	132	PHE	4.5
1	I	344	THR	4.5
1	A	272	GLU	4.5
1	E	372	ILE	4.5
1	Q	281	GLY	4.5
1	M	50	TYR	4.5
1	M	124	HIS	4.5
1	B	382	GLN	4.5
1	A	360	LEU	4.5
1	K	375	ASP	4.5
1	R	175	GLY	4.5
1	M	125	ASN	4.5
1	M	298	MET	4.5
1	N	374	CYS	4.5
1	D	9	PHE	4.5
1	E	177	LYS	4.5
1	K	364	LEU	4.5
1	I	200	GLU	4.5
1	D	363	VAL	4.5
1	J	319	PHE	4.5
1	M	64	PHE	4.5
1	G	364	LEU	4.5
1	O	308	LEU	4.5
1	L	239	TRP	4.4
1	R	229	TRP	4.4
1	E	311	ALA	4.4
1	G	213	LEU	4.4
1	Q	274	LEU	4.4
1	G	131	VAL	4.4
1	N	353	LEU	4.4
1	I	233	GLU	4.4
1	M	90	ASP	4.4
1	N	123	ASP	4.4
1	J	328	LEU	4.4
1	Q	359	GLU	4.4
1	N	289	GLY	4.4
1	Q	178	GLY	4.4
1	P	11	LYS	4.4

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Mol	Chain	Res	Type	RSRZ
1	M	341	THR	4.4
1	M	246	ILE	4.4
1	K	123	ASP	4.4
1	E	276	LYS	4.4
1	J	380	ALA	4.4
1	N	219	ALA	4.4
1	B	21	GLU	4.4
1	B	343	SER	4.4
1	L	53	TYR	4.4
1	F	326	LEU	4.4
1	N	109	HIS	4.4
1	O	306	VAL	4.4
1	P	152	CYS	4.4
1	E	317	PRO	4.3
1	I	82	LYS	4.3
1	E	137	VAL	4.3
1	L	10	VAL	4.3
1	A	117	HIS	4.3
1	N	130	GLY	4.3
1	B	8	TYR	4.3
1	E	122	LEU	4.3
1	G	212	LEU	4.3
1	A	239	TRP	4.3
1	D	161	GLU	4.3
1	Q	287	ARG	4.3
1	K	280	HIS	4.3
1	N	319	PHE	4.3
1	G	197	GLN	4.3
1	L	151	VAL	4.3
1	J	20	TRP	4.3
1	N	20	TRP	4.3
1	A	387	MET	4.3
1	M	361	VAL	4.3
1	M	142	ILE	4.3
1	O	187	LEU	4.2
1	P	328	LEU	4.2
1	C	24	LYS	4.2
1	R	114	SER	4.2
1	M	223	PRO	4.2
1	Q	297	ASN	4.2
1	Q	312	PHE	4.2
1	M	92	TYR	4.2

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Mol	Chain	Res	Type	RSRZ
1	D	381	GLY	4.2
1	D	231	ASN	4.2
1	L	315	LYS	4.2
1	L	343	SER	4.2
1	D	322	MET	4.2
1	I	274	LEU	4.2
1	L	287	ARG	4.2
1	L	339	LEU	4.2
1	M	333	THR	4.2
1	M	190	MET	4.2
1	Q	382	GLN	4.2
1	D	8	TYR	4.2
1	K	136	TYR	4.2
1	A	238	VAL	4.2
1	N	12	ASN	4.2
1	Q	292	CYS	4.2
1	B	266	ARG	4.2
1	K	54	TRP	4.2
1	D	341	THR	4.2
1	E	371	LEU	4.2
1	F	390	LYS	4.2
1	L	255	GLY	4.2
1	C	94	TYR	4.2
1	I	184	TYR	4.2
1	E	343	SER	4.2
1	L	170	SER	4.2
1	I	54	TRP	4.2
1	H	274	LEU	4.2
1	L	180	LEU	4.2
1	N	174	GLY	4.2
1	D	389	PRO	4.2
1	M	363	VAL	4.2
1	L	378	LEU	4.2
1	I	318	ARG	4.2
1	R	244	ASP	4.2
1	R	19	PRO	4.2
1	F	312	PHE	4.1
1	L	11	LYS	4.1
1	C	360	LEU	4.1
1	O	282	LEU	4.1
1	G	350	TRP	4.1
1	H	20	TRP	4.1

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Mol	Chain	Res	Type	RSRZ
1	J	160	ALA	4.1
1	L	248	VAL	4.1
1	O	62	VAL	4.1
1	Q	92	TYR	4.1
1	M	70	THR	4.1
1	J	122	LEU	4.1
1	D	11	LYS	4.1
1	G	128	VAL	4.1
1	K	40	VAL	4.1
1	B	277	GLU	4.1
1	G	61	GLY	4.1
1	L	384	ILE	4.1
1	A	180	LEU	4.1
1	I	326	LEU	4.1
1	D	266	ARG	4.1
1	B	40	VAL	4.1
1	J	385	ASP	4.1
1	N	42	ALA	4.1
1	P	278	CYS	4.1
1	L	291	ILE	4.1
1	P	9	PHE	4.1
1	Q	328	LEU	4.1
1	Q	370	LEU	4.1
1	Q	378	LEU	4.1
1	D	306	VAL	4.1
1	L	209	THR	4.1
1	M	296	THR	4.1
1	Q	333	THR	4.1
1	E	275	MET	4.1
1	I	261	PHE	4.1
1	G	124	HIS	4.1
1	O	198	LEU	4.1
1	D	28	ALA	4.1
1	Q	239	TRP	4.1
1	E	195	GLN	4.1
1	J	171	ASP	4.0
1	E	187	LEU	4.0
1	Q	237	LEU	4.0
1	P	358	ARG	4.0
1	G	184	TYR	4.0
1	H	381	GLY	4.0
1	O	257	LEU	4.0

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Mol	Chain	Res	Type	RSRZ
1	I	24	LYS	4.0
1	A	260	VAL	4.0
1	R	108	ILE	4.0
1	R	136	TYR	4.0
1	H	49	LEU	4.0
1	M	308	LEU	4.0
1	J	27	ALA	4.0
1	A	134	ASP	4.0
1	R	320	ASP	4.0
1	N	58	THR	4.0
1	A	177	LYS	4.0
1	L	319	PHE	4.0
1	I	308	LEU	4.0
1	L	274	LEU	4.0
1	C	373	ALA	4.0
1	K	28	ALA	4.0
1	K	311	ALA	4.0
1	O	104	CYS	4.0
1	N	13	ARG	4.0
1	Q	56	LYS	4.0
1	I	165	VAL	4.0
1	L	240	ILE	4.0
1	M	94	TYR	4.0
1	N	94	TYR	4.0
1	I	312	PHE	4.0
1	I	310	LEU	4.0
1	I	341	THR	4.0
1	B	72	VAL	4.0
1	G	354	GLY	4.0
1	K	382	GLN	4.0
1	N	295	PRO	4.0
1	D	123	ASP	4.0
1	K	319	PHE	4.0
1	R	350	TRP	3.9
1	D	354	GLY	3.9
1	H	332	GLY	3.9
1	C	271	VAL	3.9
1	N	167	LYS	3.9
1	M	179	ASP	3.9
1	M	241	ASN	3.9
1	K	157	MET	3.9
1	N	136	TYR	3.9

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Mol	Chain	Res	Type	RSRZ
1	G	132	PHE	3.9
1	L	93	SER	3.9
1	Q	373	ALA	3.9
1	Q	175	GLY	3.9
1	P	148	VAL	3.9
1	C	25	PHE	3.9
1	C	268	LEU	3.9
1	K	326	LEU	3.9
1	Q	34	LEU	3.9
1	Q	122	LEU	3.9
1	G	366	ASP	3.9
1	B	223	PRO	3.9
1	L	165	VAL	3.9
1	G	108	ILE	3.9
1	O	80	TYR	3.9
1	R	92	TYR	3.9
1	R	144	CYS	3.9
1	O	114	SER	3.9
1	I	378	LEU	3.9
1	N	45	LEU	3.9
1	Q	238	VAL	3.9
1	R	151	VAL	3.9
1	L	280	HIS	3.9
1	K	286	ASP	3.9
1	M	381	GLY	3.9
1	N	90	ASP	3.9
1	C	378	LEU	3.9
1	D	313	LEU	3.9
1	N	187	LEU	3.9
1	K	333	THR	3.9
1	P	70	THR	3.9
1	E	62	VAL	3.9
1	M	131	VAL	3.9
1	P	10	VAL	3.9
1	N	239	TRP	3.9
1	M	115	ASP	3.9
1	F	89	GLY	3.9
1	K	289	GLY	3.9
1	L	225	GLY	3.9
1	R	43	SER	3.9
1	F	382	GLN	3.9
1	G	274	LEU	3.9

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Mol	Chain	Res	Type	RSRZ
1	H	101	PHE	3.9
1	K	25	PHE	3.9
1	K	304	ALA	3.9
1	I	51	GLU	3.9
1	N	17	SER	3.8
1	Q	35	SER	3.8
1	M	326	LEU	3.8
1	O	312	PHE	3.8
1	M	118	PRO	3.8
1	D	96	CYS	3.8
1	M	349	ASN	3.8
1	Q	335	GLY	3.8
1	A	240	ILE	3.8
1	O	387	MET	3.8
1	B	222	TRP	3.8
1	D	187	LEU	3.8
1	G	333	THR	3.8
1	K	212	LEU	3.8
1	N	25	PHE	3.8
1	M	186	PRO	3.8
1	I	192	GLU	3.8
1	N	93	SER	3.8
1	Q	114	SER	3.8
1	D	366	ASP	3.8
1	E	286	ASP	3.8
1	Q	229	TRP	3.8
1	K	274	LEU	3.8
1	N	208	PRO	3.8
1	Q	345	TYR	3.8
1	R	261	PHE	3.8
1	N	170	SER	3.8
1	M	302	VAL	3.8
1	A	259	ALA	3.8
1	Q	317	PRO	3.8
1	B	390	LYS	3.8
1	G	312	PHE	3.8
1	H	12	ASN	3.8
1	N	203	PHE	3.8
1	O	229	TRP	3.8
1	M	114	SER	3.8
1	E	240	ILE	3.8
1	G	292	CYS	3.8

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Mol	Chain	Res	Type	RSRZ
1	G	377	LYS	3.8
1	I	67	CYS	3.8
1	N	390	LYS	3.8
1	Q	126	LYS	3.8
1	Q	113	PRO	3.8
1	R	42	ALA	3.8
1	B	264	PHE	3.8
1	N	153	LEU	3.8
1	A	50	TYR	3.8
1	F	21	GLU	3.8
1	G	78	LYS	3.8
1	D	131	VAL	3.8
1	B	12	ASN	3.8
1	H	191	ASN	3.8
1	C	228	ILE	3.8
1	M	347	ILE	3.8
1	K	160	ALA	3.7
1	N	67	CYS	3.7
1	N	213	LEU	3.7
1	M	244	ASP	3.7
1	L	226	ARG	3.7
1	N	301	VAL	3.7
1	N	41	MET	3.7
1	F	279	GLY	3.7
1	K	236	PHE	3.7
1	P	274	LEU	3.7
1	M	134	ASP	3.7
1	R	286	ASP	3.7
1	H	117	HIS	3.7
1	K	82	LYS	3.7
1	N	137	VAL	3.7
1	A	85	GLY	3.7
1	M	286	ASP	3.7
1	D	127	LEU	3.7
1	M	339	LEU	3.7
1	Q	127	LEU	3.7
1	A	345	TYR	3.7
1	G	193	LYS	3.7
1	H	390	LYS	3.7
1	Q	276	LYS	3.7
1	A	271	VAL	3.7
1	B	131	VAL	3.7

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Mol	Chain	Res	Type	RSRZ
1	G	344	THR	3.7
1	I	386	ASP	3.7
1	A	384	ILE	3.7
1	N	199	ILE	3.7
1	H	27	ALA	3.7
1	J	119	ALA	3.7
1	N	314	GLU	3.7
1	N	205	PHE	3.7
1	R	203	PHE	3.7
1	H	23	GLY	3.7
1	A	59	PRO	3.7
1	L	121	ASP	3.7
1	M	229	TRP	3.7
1	P	87	VAL	3.7
1	L	70	THR	3.7
1	H	240	ILE	3.7
1	L	265	ALA	3.7
1	D	176	LEU	3.7
1	I	212	LEU	3.7
1	N	21	GLU	3.7
1	N	371	LEU	3.7
1	R	64	PHE	3.7
1	G	375	ASP	3.6
1	L	50	TYR	3.6
1	N	271	VAL	3.6
1	O	87	VAL	3.6
1	F	67	CYS	3.6
1	P	13	ARG	3.6
1	I	108	ILE	3.6
1	C	339	LEU	3.6
1	E	339	LEU	3.6
1	F	64	PHE	3.6
1	J	210	GLY	3.6
1	M	101	PHE	3.6
1	N	261	PHE	3.6
1	D	293	THR	3.6
1	O	361	VAL	3.6
1	I	68	ILE	3.6
1	A	313	LEU	3.6
1	I	329	GLY	3.6
1	O	237	LEU	3.6
1	R	180	LEU	3.6

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Mol	Chain	Res	Type	RSRZ
1	N	44	GLN	3.6
1	C	193	LYS	3.6
1	G	179	ASP	3.6
1	E	384	ILE	3.6
1	D	139	SER	3.6
1	E	125	ASN	3.6
1	G	261	PHE	3.6
1	M	285	ASN	3.6
1	M	53	TYR	3.6
1	M	293	THR	3.6
1	N	298	MET	3.6
1	A	291	ILE	3.6
1	M	32	PRO	3.6
1	Q	277	GLU	3.6
1	D	6	GLN	3.6
1	C	76	GLY	3.6
1	Q	87	VAL	3.6
1	Q	93	SER	3.6
1	Q	249	ILE	3.6
1	A	364	LEU	3.6
1	F	308	LEU	3.6
1	K	223	PRO	3.6
1	N	269	LEU	3.6
1	P	323	LEU	3.6
1	H	319	PHE	3.6
1	E	387	MET	3.6
1	E	301	VAL	3.5
1	L	21	GLU	3.5
1	O	113	PRO	3.5
1	F	37	HIS	3.5
1	J	25	PHE	3.5
1	N	111	PHE	3.5
1	R	124	HIS	3.5
1	I	157	MET	3.5
1	L	332	GLY	3.5
1	I	26	LYS	3.5
1	K	276	LYS	3.5
1	A	168	VAL	3.5
1	L	148	VAL	3.5
1	Q	260	VAL	3.5
1	K	68	ILE	3.5
1	N	164	LEU	3.5

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Mol	Chain	Res	Type	RSRZ
1	Q	37	HIS	3.5
1	R	353	LEU	3.5
1	F	264	PHE	3.5
1	A	241	ASN	3.5
1	M	231	ASN	3.5
1	R	298	MET	3.5
1	G	137	VAL	3.5
1	M	234	LYS	3.5
1	G	326	LEU	3.5
1	O	279	GLY	3.5
1	F	298	MET	3.5
1	R	387	MET	3.5
1	B	351	ALA	3.5
1	C	340	ALA	3.5
1	D	151	VAL	3.5
1	L	92	TYR	3.5
1	O	168	VAL	3.5
1	O	290	TYR	3.5
1	M	110	HIS	3.5
1	Q	108	ILE	3.5
1	A	335	GLY	3.5
1	E	353	LEU	3.5
1	R	15	GLY	3.5
1	N	303	ARG	3.5
1	O	132	PHE	3.5
1	C	44	GLN	3.5
1	M	362	GLN	3.5
1	O	221	ASP	3.5
1	B	22	SER	3.5
1	G	337	SER	3.5
1	M	135	LYS	3.5
1	Q	380	ALA	3.5
1	F	120	PRO	3.5
1	R	208	PRO	3.5
1	N	349	ASN	3.5
1	E	91	GLU	3.5
1	D	190	MET	3.5
1	A	340	ALA	3.5
1	Q	155	PRO	3.5
1	C	321	GLU	3.5
1	M	48	GLU	3.5
1	E	142	ILE	3.4

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Mol	Chain	Res	Type	RSRZ
1	N	286	ASP	3.4
1	A	274	LEU	3.4
1	H	84	THR	3.4
1	J	378	LEU	3.4
1	M	67	CYS	3.4
1	Q	203	PHE	3.4
1	B	60	ASN	3.4
1	F	18	LYS	3.4
1	B	75	PRO	3.4
1	C	286	ASP	3.4
1	K	301	VAL	3.4
1	L	72	VAL	3.4
1	P	306	VAL	3.4
1	G	279	GLY	3.4
1	J	76	GLY	3.4
1	J	239	TRP	3.4
1	A	187	LEU	3.4
1	G	127	LEU	3.4
1	M	31	PHE	3.4
1	L	112	LYS	3.4
1	Q	374	CYS	3.4
1	R	161	GLU	3.4
1	L	284	HIS	3.4
1	E	134	ASP	3.4
1	K	259	ALA	3.4
1	P	389	PRO	3.4
1	D	76	GLY	3.4
1	D	130	GLY	3.4
1	L	57	VAL	3.4
1	B	326	LEU	3.4
1	H	360	LEU	3.4
1	K	189	THR	3.4
1	M	54	TRP	3.4
1	M	274	LEU	3.4
1	M	300	THR	3.4
1	P	282	LEU	3.4
1	P	287	ARG	3.4
1	E	109	HIS	3.4
1	E	284	HIS	3.4
1	I	316	HIS	3.4
1	B	190	MET	3.4
1	J	275	MET	3.4

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Mol	Chain	Res	Type	RSRZ
1	P	387	MET	3.4
1	L	47	LYS	3.4
1	C	240	ILE	3.4
1	I	291	ILE	3.4
1	H	257	LEU	3.4
1	O	364	LEU	3.4
1	A	121	ASP	3.4
1	H	386	ASP	3.4
1	Q	256	ASP	3.4
1	J	387	MET	3.4
1	A	193	LYS	3.4
1	M	192	GLU	3.4
1	J	40	VAL	3.4
1	I	338	SER	3.4
1	R	195	GLN	3.4
1	F	290	TYR	3.4
1	J	285	ASN	3.4
1	L	269	LEU	3.4
1	N	95	GLU	3.4
1	D	387	MET	3.4
1	E	203	PHE	3.4
1	J	101	PHE	3.4
1	C	59	PRO	3.4
1	J	19	PRO	3.4
1	Q	358	ARG	3.4
1	I	114	SER	3.4
1	M	60	ASN	3.4
1	P	131	VAL	3.4
1	A	284	HIS	3.4
1	G	82	LYS	3.4
1	I	124	HIS	3.4
1	N	66	LYS	3.4
1	R	16	HIS	3.4
1	A	173	LEU	3.4
1	I	204	LEU	3.4
1	I	213	LEU	3.4
1	P	288	LEU	3.4
1	K	381	GLY	3.4
1	R	41	MET	3.3
1	D	373	ALA	3.3
1	I	380	ALA	3.3
1	C	52	LYS	3.3

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Mol	Chain	Res	Type	RSRZ
1	K	112	LYS	3.3
1	A	148	VAL	3.3
1	C	128	VAL	3.3
1	F	271	VAL	3.3
1	H	361	VAL	3.3
1	L	238	VAL	3.3
1	Q	368	VAL	3.3
1	E	309	ARG	3.3
1	R	58	THR	3.3
1	D	94	TYR	3.3
1	A	203	PHE	3.3
1	K	377	LYS	3.3
1	Q	95	GLU	3.3
1	D	320	ASP	3.3
1	I	139	SER	3.3
1	A	165	VAL	3.3
1	A	248	VAL	3.3
1	K	306	VAL	3.3
1	O	128	VAL	3.3
1	J	15	GLY	3.3
1	E	374	CYS	3.3
1	G	291	ILE	3.3
1	K	357	GLU	3.3
1	M	26	LYS	3.3
1	Q	390	LYS	3.3
1	G	353	LEU	3.3
1	I	282	LEU	3.3
1	O	328	LEU	3.3
1	G	60	ASN	3.3
1	G	191	ASN	3.3
1	I	342	ASP	3.3
1	P	261	PHE	3.3
1	J	383	SER	3.3
1	B	124	HIS	3.3
1	I	149	LYS	3.3
1	C	199	ILE	3.3
1	N	184	TYR	3.3
1	N	320	ASP	3.3
1	L	275	MET	3.3
1	I	25	PHE	3.3
1	I	193	LYS	3.3
1	I	280	HIS	3.3

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Mol	Chain	Res	Type	RSRZ
1	J	277	GLU	3.3
1	M	27	ALA	3.3
1	N	380	ALA	3.3
1	R	18	LYS	3.3
1	E	150	GLY	3.3
1	F	293	THR	3.3
1	K	344	THR	3.3
1	H	57	VAL	3.3
1	I	40	VAL	3.3
1	K	137	VAL	3.3
1	L	131	VAL	3.3
1	M	301	VAL	3.3
1	R	54	TRP	3.3
1	G	286	ASP	3.3
1	N	309	ARG	3.3
1	C	47	LYS	3.3
1	H	53	TYR	3.3
1	H	136	TYR	3.3
1	J	11	LYS	3.3
1	M	353	LEU	3.3
1	O	288	LEU	3.3
1	N	80	TYR	3.3
1	C	31	PHE	3.3
1	L	156	ALA	3.3
1	L	218	CYS	3.3
1	M	178	GLY	3.3
1	B	358	ARG	3.3
1	L	318	ARG	3.3
1	C	134	ASP	3.3
1	D	137	VAL	3.3
1	D	201	ASP	3.3
1	G	385	ASP	3.3
1	H	134	ASP	3.3
1	J	151	VAL	3.3
1	P	40	VAL	3.3
1	R	12	ASN	3.3
1	G	68	ILE	3.3
1	Q	204	LEU	3.3
1	J	88	PHE	3.3
1	K	312	PHE	3.3
1	B	4	ALA	3.3
1	O	219	ALA	3.3

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Mol	Chain	Res	Type	RSRZ
1	F	52	LYS	3.3
1	L	174	GLY	3.3
1	M	390	LYS	3.3
1	C	125	ASN	3.3
1	M	342	ASP	3.3
1	R	260	VAL	3.2
1	N	348	SER	3.2
1	D	291	ILE	3.2
1	P	204	LEU	3.2
1	Q	308	LEU	3.2
1	D	283	MET	3.2
1	J	136	TYR	3.2
1	O	298	MET	3.2
1	A	321	GLU	3.2
1	A	374	CYS	3.2
1	G	368	VAL	3.2
1	O	238	VAL	3.2
1	I	337	SER	3.2
1	R	155	PRO	3.2
1	A	390	LYS	3.2
1	D	220	ARG	3.2
1	A	371	LEU	3.2
1	E	54	TRP	3.2
1	H	192	GLU	3.2
1	R	228	ILE	3.2
1	B	94	TYR	3.2
1	D	15	GLY	3.2
1	L	80	TYR	3.2
1	O	134	ASP	3.2
1	N	382	GLN	3.2
1	E	376	LYS	3.2
1	R	167	LYS	3.2
1	E	361	VAL	3.2
1	L	48	GLU	3.2
1	O	148	VAL	3.2
1	A	385	ASP	3.2
1	I	288	LEU	3.2
1	N	244	ASP	3.2
1	P	187	LEU	3.2
1	Q	221	ASP	3.2
1	M	297	ASN	3.2
1	Q	130	GLY	3.2

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Mol	Chain	Res	Type	RSRZ
1	E	185	TYR	3.2
1	Q	111	PHE	3.2
1	G	133	GLU	3.2
1	L	314	GLU	3.2
1	M	344	THR	3.2
1	R	277	GLU	3.2
1	H	159	ARG	3.2
1	A	109	HIS	3.2
1	B	139	SER	3.2
1	B	284	HIS	3.2
1	C	343	SER	3.2
1	M	317	PRO	3.2
1	R	295	PRO	3.2
1	A	368	VAL	3.2
1	P	365	VAL	3.2
1	R	279	GLY	3.2
1	A	24	LYS	3.2
1	H	246	ILE	3.2
1	K	198	LEU	3.2
1	K	353	LEU	3.2
1	O	213	LEU	3.2
1	R	269	LEU	3.2
1	M	119	ALA	3.2
1	I	132	PHE	3.2
1	A	343	SER	3.2
1	L	230	HIS	3.2
1	M	316	HIS	3.2
1	H	113	PRO	3.2
1	K	32	PRO	3.2
1	M	194	ASP	3.2
1	K	206	GLU	3.2
1	M	95	GLU	3.2
1	I	353	LEU	3.2
1	J	313	LEU	3.2
1	R	278	CYS	3.2
1	A	172	ALA	3.2
1	K	264	PHE	3.2
1	R	63	THR	3.2
1	B	149	LYS	3.2
1	E	26	LYS	3.2
1	O	36	LYS	3.2
1	B	317	PRO	3.2

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Mol	Chain	Res	Type	RSRZ
1	Q	208	PRO	3.2
1	L	191	ASN	3.2
1	H	271	VAL	3.2
1	B	187	LEU	3.1
1	E	246	ILE	3.1
1	E	291	ILE	3.1
1	J	384	ILE	3.1
1	A	215	THR	3.1
1	N	264	PHE	3.1
1	R	337	SER	3.1
1	N	54	TRP	3.1
1	M	238	VAL	3.1
1	N	248	VAL	3.1
1	P	169	VAL	3.1
1	E	199	ILE	3.1
1	E	323	LEU	3.1
1	H	359	GLU	3.1
1	H	382	GLN	3.1
1	N	372	ILE	3.1
1	R	328	LEU	3.1
1	A	181	ALA	3.1
1	E	385	ASP	3.1
1	G	181	ALA	3.1
1	P	383	SER	3.1
1	G	214	THR	3.1
1	J	111	PHE	3.1
1	Q	77	ASN	3.1
1	Q	188	THR	3.1
1	Q	231	ASN	3.1
1	C	144	CYS	3.1
1	I	50	TYR	3.1
1	M	290	TYR	3.1
1	C	116	LYS	3.1
1	O	54	TRP	3.1
1	L	168	VAL	3.1
1	Q	151	VAL	3.1
1	Q	306	VAL	3.1
1	G	123	ASP	3.1
1	A	127	LEU	3.1
1	K	204	LEU	3.1
1	L	124	HIS	3.1
1	A	373	ALA	3.1

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Mol	Chain	Res	Type	RSRZ
1	D	384	ILE	3.1
1	O	199	ILE	3.1
1	Q	313	LEU	3.1
1	E	358	ARG	3.1
1	I	27	ALA	3.1
1	M	191	ASN	3.1
1	C	312	PHE	3.1
1	E	234	LYS	3.1
1	G	223	PRO	3.1
1	F	334	GLY	3.1
1	F	248	VAL	3.1
1	J	137	VAL	3.1
1	K	221	ASP	3.1
1	M	128	VAL	3.1
1	O	165	VAL	3.1
1	N	245	HIS	3.1
1	I	370	LEU	3.1
1	K	24	LYS	3.1
1	K	328	LEU	3.1
1	Q	388	ILE	3.1
1	A	129	GLY	3.1
1	A	225	GLY	3.1
1	D	79	PHE	3.1
1	G	64	PHE	3.1
1	I	179	ASP	3.1
1	B	355	LYS	3.1
1	N	96	CYS	3.1
1	I	271	VAL	3.1
1	N	260	VAL	3.1
1	N	368	VAL	3.1
1	O	248	VAL	3.1
1	O	368	VAL	3.1
1	R	169	VAL	3.1
1	M	322	MET	3.1
1	A	153	LEU	3.1
1	B	313	LEU	3.1
1	G	257	LEU	3.1
1	H	353	LEU	3.1
1	I	340	ALA	3.1
1	K	340	ALA	3.1
1	P	181	ALA	3.1
1	P	313	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
1	D	182	GLY	3.1
1	F	101	PHE	3.1
1	E	136	TYR	3.1
1	N	92	TYR	3.1
1	O	185	TYR	3.1
1	A	72	VAL	3.1
1	E	260	VAL	3.1
1	L	104	CYS	3.1
1	L	283	MET	3.1
1	A	353	LEU	3.1
1	D	378	LEU	3.1
1	H	160	ALA	3.1
1	M	176	LEU	3.1
1	Q	172	ALA	3.1
1	Q	310	LEU	3.1
1	R	326	LEU	3.1
1	Q	295	PRO	3.1
1	R	113	PRO	3.1
1	K	261	PHE	3.0
1	E	241	ASN	3.0
1	J	280	HIS	3.0
1	R	230	HIS	3.0
1	K	197	GLN	3.0
1	H	10	VAL	3.0
1	P	23	GLY	3.0
1	B	58	THR	3.0
1	B	140	CYS	3.0
1	D	317	PRO	3.0
1	G	313	LEU	3.0
1	J	155	PRO	3.0
1	J	389	PRO	3.0
1	L	115	ASP	3.0
1	M	350	TRP	3.0
1	E	369	ASN	3.0
1	F	191	ASN	3.0
1	J	312	PHE	3.0
1	B	97	TYR	3.0
1	E	262	SER	3.0
1	H	337	SER	3.0
1	K	35	SER	3.0
1	M	136	TYR	3.0
1	N	345	TYR	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	145	GLY	3.0
1	L	210	GLY	3.0
1	H	171	ASP	3.0
1	R	302	VAL	3.0
1	C	323	LEU	3.0
1	D	360	LEU	3.0
1	H	333	THR	3.0
1	K	46	THR	3.0
1	N	59	PRO	3.0
1	Q	339	LEU	3.0
1	Q	344	THR	3.0
1	A	125	ASN	3.0
1	A	144	CYS	3.0
1	J	142	ILE	3.0
1	K	229	TRP	3.0
1	I	236	PHE	3.0
1	O	261	PHE	3.0
1	R	319	PHE	3.0
1	C	185	TYR	3.0
1	M	227	GLY	3.0
1	D	58	THR	3.0
1	N	75	PRO	3.0
1	Q	154	PRO	3.0
1	F	153	LEU	3.0
1	F	311	ALA	3.0
1	N	257	LEU	3.0
1	O	340	ALA	3.0
1	Q	176	LEU	3.0
1	N	249	ILE	3.0
1	L	20	TRP	3.0
1	O	358	ARG	3.0
1	G	25	PHE	3.0
1	M	132	PHE	3.0
1	P	111	PHE	3.0
1	G	320	ASP	3.0
1	O	115	ASP	3.0
1	C	150	GLY	3.0
1	J	381	GLY	3.0
1	A	26	LYS	3.0
1	B	26	LYS	3.0
1	I	345	TYR	3.0
1	J	390	LYS	3.0

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Mol	Chain	Res	Type	RSRZ
1	N	78	LYS	3.0
1	N	151	VAL	3.0
1	N	168	VAL	3.0
1	F	373	ALA	3.0
1	J	172	ALA	3.0
1	M	42	ALA	3.0
1	G	280	HIS	3.0
1	Q	316	HIS	3.0
1	F	388	ILE	3.0
1	O	246	ILE	3.0
1	B	132	PHE	3.0
1	J	29	ASP	3.0
1	M	383	SER	3.0
1	N	158	SER	3.0
1	M	319	PHE	3.0
1	A	334	GLY	3.0
1	C	374	CYS	3.0
1	L	61	GLY	3.0
1	M	292	CYS	3.0
1	P	135	LYS	3.0
1	R	23	GLY	3.0
1	A	195	GLN	3.0
1	Q	53	TYR	3.0
1	Q	120	PRO	3.0
1	G	298	MET	3.0
1	A	124	HIS	3.0
1	J	189	THR	3.0
1	N	296	THR	3.0
1	E	172	ALA	3.0
1	N	311	ALA	3.0
1	G	204	LEU	3.0
1	K	213	LEU	3.0
1	Q	213	LEU	3.0
1	D	35	SER	3.0
1	J	33	ASP	3.0
1	M	356	SER	3.0
1	O	347	ILE	3.0
1	Q	228	ILE	3.0
1	I	350	TRP	3.0
1	N	350	TRP	3.0
1	D	118	PRO	2.9
1	C	361	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	298	MET	2.9
1	G	58	THR	2.9
1	J	87	VAL	2.9
1	M	181	ALA	2.9
1	Q	168	VAL	2.9
1	F	339	LEU	2.9
1	L	346	ASP	2.9
1	M	49	LEU	2.9
1	R	45	LEU	2.9
1	R	164	LEU	2.9
1	D	252	GLN	2.9
1	E	174	GLY	2.9
1	G	281	GLY	2.9
1	Q	254	GLY	2.9
1	G	309	ARG	2.9
1	K	191	ASN	2.9
1	M	159	ARG	2.9
1	N	100	PHE	2.9
1	A	258	LYS	2.9
1	G	222	TRP	2.9
1	J	54	TRP	2.9
1	O	32	PRO	2.9
1	A	196	GLU	2.9
1	E	322	MET	2.9
1	H	275	MET	2.9
1	E	271	VAL	2.9
1	L	271	VAL	2.9
1	E	127	LEU	2.9
1	G	35	SER	2.9
1	K	153	LEU	2.9
1	K	180	LEU	2.9
1	Q	383	SER	2.9
1	C	227	GLY	2.9
1	H	145	GLY	2.9
1	M	226	ARG	2.9
1	D	199	ILE	2.9
1	D	249	ILE	2.9
1	P	142	ILE	2.9
1	Q	347	ILE	2.9
1	E	208	PRO	2.9
1	N	37	HIS	2.9
1	L	134	ASP	2.9

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Mol	Chain	Res	Type	RSRZ
1	M	366	ASP	2.9
1	O	239	TRP	2.9
1	P	54	TRP	2.9
1	B	380	ALA	2.9
1	E	94	TYR	2.9
1	E	140	CYS	2.9
1	E	248	VAL	2.9
1	F	40	VAL	2.9
1	H	151	VAL	2.9
1	J	301	VAL	2.9
1	L	383	SER	2.9
1	K	294	CYS	2.9
1	N	315	LYS	2.9
1	O	152	CYS	2.9
1	E	61	GLY	2.9
1	J	74	ASN	2.9
1	Q	82	LYS	2.9
1	Q	353	LEU	2.9
1	C	384	ILE	2.9
1	J	388	ILE	2.9
1	R	291	ILE	2.9
1	G	233	GLU	2.9
1	G	357	GLU	2.9
1	F	385	ASP	2.9
1	H	88	PHE	2.9
1	I	123	ASP	2.9
1	P	25	PHE	2.9
1	R	100	PHE	2.9
1	C	208	PRO	2.9
1	E	197	GLN	2.9
1	K	389	PRO	2.9
1	L	13	ARG	2.9
1	B	84	THR	2.9
1	L	78	LYS	2.9
1	H	43	SER	2.9
1	E	351	ALA	2.9
1	I	57	VAL	2.9
1	O	164	LEU	2.9
1	A	142	ILE	2.9
1	N	134	ASP	2.9
1	A	358	ARG	2.9
1	D	124	HIS	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	31	PHE	2.9
1	M	138	LYS	2.9
1	N	120	PRO	2.9
1	R	205	PHE	2.9
1	A	262	SER	2.9
1	C	91	GLU	2.9
1	E	58	THR	2.9
1	C	241	ASN	2.9
1	F	343	SER	2.9
1	G	232	ASN	2.9
1	K	379	GLU	2.9
1	E	259	ALA	2.9
1	K	373	ALA	2.9
1	M	151	VAL	2.9
1	R	239	TRP	2.9
1	I	269	LEU	2.9
1	M	213	LEU	2.9
1	L	56	LYS	2.9
1	O	83	LYS	2.9
1	C	291	ILE	2.9
1	G	372	ILE	2.9
1	L	117	HIS	2.9
1	P	228	ILE	2.9
1	Q	280	HIS	2.9
1	A	154	PRO	2.9
1	B	9	PHE	2.9
1	C	101	PHE	2.9
1	L	31	PHE	2.9
1	N	236	PHE	2.9
1	R	88	PHE	2.9
1	A	63	THR	2.9
1	E	279	GLY	2.9
1	M	188	THR	2.9
1	R	70	THR	2.9
1	A	275	MET	2.9
1	M	275	MET	2.9
1	Q	41	MET	2.9
1	I	259	ALA	2.9
1	D	14	VAL	2.9
1	D	386	ASP	2.9
1	I	306	VAL	2.9
1	J	365	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
1	K	290	TYR	2.9
1	D	326	LEU	2.8
1	F	310	LEU	2.8
1	N	34	LEU	2.8
1	N	282	LEU	2.8
1	B	120	PRO	2.8
1	F	389	PRO	2.8
1	P	120	PRO	2.8
1	P	191	ASN	2.8
1	P	101	PHE	2.8
1	I	381	GLY	2.8
1	J	61	GLY	2.8
1	Q	66	LYS	2.8
1	Q	145	GLY	2.8
1	G	151	VAL	2.8
1	D	290	TYR	2.8
1	G	97	TYR	2.8
1	G	110	HIS	2.8
1	K	128	VAL	2.8
1	O	169	VAL	2.8
1	O	365	VAL	2.8
1	R	284	HIS	2.8
1	R	361	VAL	2.8
1	H	371	LEU	2.8
1	N	378	LEU	2.8
1	O	92	TYR	2.8
1	P	364	LEU	2.8
1	R	204	LEU	2.8
1	H	350	TRP	2.8
1	I	222	TRP	2.8
1	O	208	PRO	2.8
1	P	291	ILE	2.8
1	K	143	ARG	2.8
1	R	85	GLY	2.8
1	F	188	THR	2.8
1	G	171	ASP	2.8
1	L	194	ASP	2.8
1	O	374	CYS	2.8
1	R	96	CYS	2.8
1	P	275	MET	2.8
1	A	365	VAL	2.8
1	D	330	LYS	2.8

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Mol	Chain	Res	Type	RSRZ
1	R	87	VAL	2.8
1	R	276	LYS	2.8
1	C	176	LEU	2.8
1	K	77	ASN	2.8
1	N	308	LEU	2.8
1	F	20	TRP	2.8
1	M	239	TRP	2.8
1	O	223	PRO	2.8
1	F	329	GLY	2.8
1	K	182	GLY	2.8
1	L	381	GLY	2.8
1	Q	139	SER	2.8
1	Q	272	GLU	2.8
1	G	386	ASP	2.8
1	K	203	PHE	2.8
1	L	189	THR	2.8
1	M	46	THR	2.8
1	P	88	PHE	2.8
1	P	300	THR	2.8
1	B	16	HIS	2.8
1	F	16	HIS	2.8
1	I	265	ALA	2.8
1	K	211	ALA	2.8
1	L	67	CYS	2.8
1	R	304	ALA	2.8
1	A	369	ASN	2.8
1	G	148	VAL	2.8
1	H	365	VAL	2.8
1	O	137	VAL	2.8
1	Q	72	VAL	2.8
1	A	200	GLU	2.8
1	G	192	GLU	2.8
1	B	19	PRO	2.8
1	H	92	TYR	2.8
1	K	92	TYR	2.8
1	M	122	LEU	2.8
1	M	184	TYR	2.8
1	P	371	LEU	2.8
1	C	354	GLY	2.8
1	L	329	GLY	2.8
1	P	286	ASP	2.8
1	B	54	TRP	2.8

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Mol	Chain	Res	Type	RSRZ
1	N	229	TRP	2.8
1	B	236	PHE	2.8
1	C	296	THR	2.8
1	H	63	THR	2.8
1	P	64	PHE	2.8
1	R	333	THR	2.8
1	M	230	HIS	2.8
1	N	284	HIS	2.8
1	F	41	MET	2.8
1	G	48	GLU	2.8
1	M	233	GLU	2.8
1	L	278	CYS	2.8
1	B	365	VAL	2.8
1	G	40	VAL	2.8
1	J	248	VAL	2.8
1	C	313	LEU	2.8
1	G	187	LEU	2.8
1	D	355	LYS	2.8
1	H	120	PRO	2.8
1	I	313	LEU	2.8
1	K	186	PRO	2.8
1	L	153	LEU	2.8
1	M	257	LEU	2.8
1	N	173	LEU	2.8
1	P	92	TYR	2.8
1	P	305	SER	2.8
1	Q	268	LEU	2.8
1	E	345	TYR	2.8
1	R	97	TYR	2.8
1	B	347	ILE	2.8
1	R	246	ILE	2.8
1	A	344	THR	2.8
1	C	100	PHE	2.8
1	D	203	PHE	2.8
1	J	31	PHE	2.8
1	O	272	GLU	2.8
1	M	263	ARG	2.8
1	L	369	ASN	2.8
1	I	219	ALA	2.8
1	R	28	ALA	2.8
1	R	211	ALA	2.8
1	C	123	ASP	2.8

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Mol	Chain	Res	Type	RSRZ
1	I	33	ASP	2.8
1	R	177	LYS	2.8
1	C	186	PRO	2.8
1	C	262	SER	2.8
1	E	57	VAL	2.8
1	E	168	VAL	2.8
1	G	168	VAL	2.8
1	H	169	VAL	2.8
1	I	260	VAL	2.8
1	R	131	VAL	2.8
1	D	374	CYS	2.8
1	H	278	CYS	2.8
1	I	164	LEU	2.8
1	M	364	LEU	2.8
1	O	269	LEU	2.8
1	E	133	GLU	2.8
1	R	359	GLU	2.8
1	C	246	ILE	2.8
1	O	291	ILE	2.8
1	R	296	THR	2.8
1	B	116	LYS	2.7
1	J	100	PHE	2.7
1	N	24	LYS	2.7
1	A	386	ASP	2.7
1	P	179	ASP	2.7
1	Q	123	ASP	2.7
1	E	321	GLU	2.7
1	P	22	SER	2.7
1	K	363	VAL	2.7
1	M	120	PRO	2.7
1	B	378	LEU	2.7
1	M	378	LEU	2.7
1	Q	153	LEU	2.7
1	Q	269	LEU	2.7
1	B	278	CYS	2.7
1	C	290	TYR	2.7
1	G	94	TYR	2.7
1	I	290	TYR	2.7
1	J	50	TYR	2.7
1	A	230	HIS	2.7
1	B	280	HIS	2.7
1	C	177	LYS	2.7

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Mol	Chain	Res	Type	RSRZ
1	F	384	ILE	2.7
1	G	231	ASN	2.7
1	N	47	LYS	2.7
1	N	376	LYS	2.7
1	Q	235	ASN	2.7
1	R	388	ILE	2.7
1	K	121	ASP	2.7
1	M	111	PHE	2.7
1	P	312	PHE	2.7
1	C	298	MET	2.7
1	O	275	MET	2.7
1	Q	351	ALA	2.7
1	K	158	SER	2.7
1	M	289	GLY	2.7
1	A	363	VAL	2.7
1	E	148	VAL	2.7
1	N	302	VAL	2.7
1	D	213	LEU	2.7
1	M	268	LEU	2.7
1	K	235	ASN	2.7
1	O	307	HIS	2.7
1	Q	284	HIS	2.7
1	J	345	TYR	2.7
1	A	256	ASP	2.7
1	D	51	GLU	2.7
1	L	123	ASP	2.7
1	M	68	ILE	2.7
1	D	67	CYS	2.7
1	H	294	CYS	2.7
1	M	385	ASP	2.7
1	Q	48	GLU	2.7
1	C	264	PHE	2.7
1	L	111	PHE	2.7
1	C	367	GLY	2.7
1	J	159	ARG	2.7
1	A	116	LYS	2.7
1	B	27	ALA	2.7
1	N	76	GLY	2.7
1	B	126	LYS	2.7
1	G	149	LYS	2.7
1	L	362	GLN	2.7
1	Q	75	PRO	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	37	HIS	2.7
1	E	368	VAL	2.7
1	N	361	VAL	2.7
1	F	378	LEU	2.7
1	H	268	LEU	2.7
1	I	268	LEU	2.7
1	M	237	LEU	2.7
1	Q	212	LEU	2.7
1	A	65	ASP	2.7
1	K	115	ASP	2.7
1	Q	90	ASP	2.7
1	B	333	THR	2.7
1	A	150	GLY	2.7
1	M	278	CYS	2.7
1	O	294	CYS	2.7
1	R	225	GLY	2.7
1	C	119	ALA	2.7
1	F	322	MET	2.7
1	J	43	SER	2.7
1	A	186	PRO	2.7
1	C	389	PRO	2.7
1	E	336	GLU	2.7
1	K	349	ASN	2.7
1	O	99	GLU	2.7
1	E	238	VAL	2.7
1	A	45	LEU	2.7
1	C	164	LEU	2.7
1	C	353	LEU	2.7
1	C	370	LEU	2.7
1	D	257	LEU	2.7
1	D	276	LYS	2.7
1	G	98	LYS	2.7
1	I	127	LEU	2.7
1	Q	326	LEU	2.7
1	F	228	ILE	2.7
1	L	372	ILE	2.7
1	J	175	GLY	2.7
1	M	382	GLN	2.7
1	N	61	GLY	2.7
1	P	354	GLY	2.7
1	E	139	SER	2.7
1	A	312	PHE	2.7

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Mol	Chain	Res	Type	RSRZ
1	E	272	GLU	2.7
1	I	64	PHE	2.7
1	I	277	GLU	2.7
1	M	147	SER	2.7
1	N	338	SER	2.7
1	M	312	PHE	2.7
1	A	304	ALA	2.7
1	C	278	CYS	2.7
1	H	60	ASN	2.7
1	H	369	ASN	2.7
1	L	30	ASN	2.7
1	R	104	CYS	2.7
1	I	377	LYS	2.7
1	K	253	LYS	2.7
1	M	98	LYS	2.7
1	Q	386	ASP	2.7
1	B	137	VAL	2.7
1	B	213	LEU	2.7
1	C	137	VAL	2.7
1	F	54	TRP	2.7
1	G	268	LEU	2.7
1	N	127	LEU	2.7
1	O	204	LEU	2.7
1	B	281	GLY	2.7
1	D	142	ILE	2.7
1	E	93	SER	2.7
1	F	94	TYR	2.7
1	L	114	SER	2.7
1	M	216	SER	2.7
1	M	262	SER	2.7
1	R	262	SER	2.7
1	L	38	ASN	2.7
1	B	42	ALA	2.7
1	E	342	ASP	2.7
1	I	41	MET	2.7
1	K	322	MET	2.7
1	L	64	PHE	2.7
1	M	311	ALA	2.7
1	N	342	ASP	2.7
1	O	311	ALA	2.7
1	R	56	LYS	2.7
1	N	179	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
1	E	359	GLU	2.6
1	G	196	GLU	2.6
1	O	382	GLN	2.6
1	C	72	VAL	2.6
1	D	72	VAL	2.6
1	D	128	VAL	2.6
1	O	378	LEU	2.6
1	Q	62	VAL	2.6
1	E	188	THR	2.6
1	L	217	GLY	2.6
1	N	89	GLY	2.6
1	N	255	GLY	2.6
1	R	145	GLY	2.6
1	L	147	SER	2.6
1	O	276	LYS	2.6
1	Q	325	LYS	2.6
1	G	249	ILE	2.6
1	N	384	ILE	2.6
1	I	375	ASP	2.6
1	J	194	ASP	2.6
1	N	385	ASP	2.6
1	O	184	TYR	2.6
1	C	322	MET	2.6
1	H	25	PHE	2.6
1	H	110	HIS	2.6
1	H	264	PHE	2.6
1	P	304	ALA	2.6
1	L	197	GLN	2.6
1	J	96	CYS	2.6
1	C	364	LEU	2.6
1	E	173	LEU	2.6
1	E	313	LEU	2.6
1	F	62	VAL	2.6
1	G	267	GLY	2.6
1	M	360	LEU	2.6
1	N	57	VAL	2.6
1	O	72	VAL	2.6
1	Q	137	VAL	2.6
1	R	165	VAL	2.6
1	A	356	SER	2.6
1	I	383	SER	2.6
1	N	383	SER	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	123	ASP	2.6
1	F	291	ILE	2.6
1	E	230	HIS	2.6
1	K	48	GLU	2.6
1	F	208	PRO	2.6
1	J	92	TYR	2.6
1	K	345	TYR	2.6
1	O	97	TYR	2.6
1	O	295	PRO	2.6
1	G	211	ALA	2.6
1	K	31	PHE	2.6
1	L	172	ALA	2.6
1	N	275	MET	2.6
1	P	119	ALA	2.6
1	Q	64	PHE	2.6
1	Q	132	PHE	2.6
1	R	340	ALA	2.6
1	D	126	LYS	2.6
1	Q	289	GLY	2.6
1	B	164	LEU	2.6
1	G	43	SER	2.6
1	H	212	LEU	2.6
1	I	72	VAL	2.6
1	I	180	LEU	2.6
1	J	168	VAL	2.6
1	K	188	THR	2.6
1	N	62	VAL	2.6
1	N	328	LEU	2.6
1	Q	170	SER	2.6
1	R	137	VAL	2.6
1	N	140	CYS	2.6
1	Q	144	CYS	2.6
1	I	382	GLN	2.6
1	A	199	ILE	2.6
1	C	229	TRP	2.6
1	J	246	ILE	2.6
1	M	199	ILE	2.6
1	P	239	TRP	2.6
1	P	284	HIS	2.6
1	N	155	PRO	2.6
1	A	311	ALA	2.6
1	E	25	PHE	2.6

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Mol	Chain	Res	Type	RSRZ
1	O	236	PHE	2.6
1	Q	101	PHE	2.6
1	Q	236	PHE	2.6
1	D	279	GLY	2.6
1	G	270	GLU	2.6
1	I	125	ASN	2.6
1	O	145	GLY	2.6
1	P	299	GLY	2.6
1	B	244	ASP	2.6
1	D	343	SER	2.6
1	H	70	THR	2.6
1	N	46	THR	2.6
1	P	188	THR	2.6
1	K	370	LEU	2.6
1	L	382	GLN	2.6
1	B	167	LYS	2.6
1	I	78	LYS	2.6
1	P	36	LYS	2.6
1	C	86	CYS	2.6
1	H	152	CYS	2.6
1	H	142	ILE	2.6
1	K	384	ILE	2.6
1	P	246	ILE	2.6
1	B	136	TYR	2.6
1	C	351	ALA	2.6
1	D	251	MET	2.6
1	F	119	ALA	2.6
1	B	101	PHE	2.6
1	D	277	GLU	2.6
1	I	101	PHE	2.6
1	A	342	ASP	2.6
1	I	130	GLY	2.6
1	R	227	GLY	2.6
1	G	250	SER	2.6
1	L	390	LYS	2.6
1	O	63	THR	2.6
1	A	268	LEU	2.6
1	B	128	VAL	2.6
1	D	260	VAL	2.6
1	E	306	VAL	2.6
1	F	14	VAL	2.6
1	G	230	HIS	2.6

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Mol	Chain	Res	Type	RSRZ
1	L	370	LEU	2.6
1	E	295	PRO	2.6
1	G	59	PRO	2.6
1	N	272	GLU	2.6
1	O	118	PRO	2.6
1	R	120	PRO	2.6
1	R	379	GLU	2.6
1	A	347	ILE	2.6
1	K	105	ILE	2.6
1	E	181	ALA	2.6
1	D	101	PHE	2.6
1	E	101	PHE	2.6
1	F	386	ASP	2.6
1	I	298	MET	2.6
1	H	54	TRP	2.6
1	K	30	ASN	2.6
1	L	27	ALA	2.6
1	L	385	ASP	2.6
1	M	25	PHE	2.6
1	M	81	GLY	2.6
1	N	335	GLY	2.6
1	O	385	ASP	2.6
1	N	300	THR	2.6
1	D	206	GLU	2.6
1	F	124	HIS	2.6
1	M	117	HIS	2.6
1	Q	307	HIS	2.6
1	A	302	VAL	2.6
1	D	165	VAL	2.6
1	G	287	ARG	2.6
1	G	370	LEU	2.6
1	J	13	ARG	2.6
1	K	57	VAL	2.6
1	K	320	ASP	2.5
1	P	388	ILE	2.5
1	Q	134	ASP	2.5
1	E	367	GLY	2.5
1	G	332	GLY	2.5
1	I	299	GLY	2.5
1	M	334	GLY	2.5
1	N	157	MET	2.5
1	F	132	PHE	2.5

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Mol	Chain	Res	Type	RSRZ
1	I	97	TYR	2.5
1	L	97	TYR	2.5
1	P	140	CYS	2.5
1	Q	140	CYS	2.5
1	D	222	TRP	2.5
1	I	196	GLU	2.5
1	R	95	GLU	2.5
1	D	316	HIS	2.5
1	P	37	HIS	2.5
1	M	116	LYS	2.5
1	O	116	LYS	2.5
1	B	268	LEU	2.5
1	F	164	LEU	2.5
1	G	176	LEU	2.5
1	L	282	LEU	2.5
1	O	153	LEU	2.5
1	O	260	VAL	2.5
1	Q	371	LEU	2.5
1	B	7	ASP	2.5
1	C	232	ASN	2.5
1	E	179	ASP	2.5
1	J	386	ASP	2.5
1	R	179	ASP	2.5
1	C	255	GLY	2.5
1	D	335	GLY	2.5
1	L	254	GLY	2.5
1	L	28	ALA	2.5
1	M	251	MET	2.5
1	M	259	ALA	2.5
1	Q	42	ALA	2.5
1	Q	314	GLU	2.5
1	Q	384	ILE	2.5
1	A	139	SER	2.5
1	B	11	LYS	2.5
1	B	79	PHE	2.5
1	B	203	PHE	2.5
1	D	264	PHE	2.5
1	H	312	PHE	2.5
1	K	80	TYR	2.5
1	M	261	PHE	2.5
1	N	312	PHE	2.5
1	A	292	CYS	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	230	HIS	2.5
1	E	350	TRP	2.5
1	F	84	THR	2.5
1	G	229	TRP	2.5
1	G	293	THR	2.5
1	J	209	THR	2.5
1	L	344	THR	2.5
1	L	374	CYS	2.5
1	C	368	VAL	2.5
1	G	271	VAL	2.5
1	H	75	PRO	2.5
1	I	231	ASN	2.5
1	K	176	LEU	2.5
1	L	34	LEU	2.5
1	L	137	VAL	2.5
1	L	257	LEU	2.5
1	M	365	VAL	2.5
1	N	49	LEU	2.5
1	O	120	PRO	2.5
1	O	363	VAL	2.5
1	P	180	LEU	2.5
1	R	10	VAL	2.5
1	R	268	LEU	2.5
1	G	272	GLU	2.5
1	I	254	GLY	2.5
1	K	149	LYS	2.5
1	F	111	PHE	2.5
1	M	284	HIS	2.5
1	O	316	HIS	2.5
1	G	290	TYR	2.5
1	M	97	TYR	2.5
1	O	53	TYR	2.5
1	P	94	TYR	2.5
1	Q	290	TYR	2.5
1	B	293	THR	2.5
1	F	341	THR	2.5
1	I	188	THR	2.5
1	M	161	GLU	2.5
1	P	33	ASP	2.5
1	A	294	CYS	2.5
1	M	222	TRP	2.5
1	Q	91	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	389	PRO	2.5
1	B	62	VAL	2.5
1	B	269	LEU	2.5
1	C	306	VAL	2.5
1	E	257	LEU	2.5
1	F	282	LEU	2.5
1	F	335	GLY	2.5
1	H	174	GLY	2.5
1	H	260	VAL	2.5
1	H	281	GLY	2.5
1	I	174	GLY	2.5
1	I	93	SER	2.5
1	P	199	ILE	2.5
1	C	362	GLN	2.5
1	P	316	HIS	2.5
1	C	79	PHE	2.5
1	F	244	ASP	2.5
1	Q	79	PHE	2.5
1	K	214	THR	2.5
1	L	296	THR	2.5
1	M	369	ASN	2.5
1	N	84	THR	2.5
1	Q	84	THR	2.5
1	F	358	ARG	2.5
1	F	118	PRO	2.5
1	C	54	TRP	2.5
1	C	145	GLY	2.5
1	C	173	LEU	2.5
1	F	274	LEU	2.5
1	F	350	TRP	2.5
1	H	34	LEU	2.5
1	I	365	VAL	2.5
1	K	187	LEU	2.5
1	P	57	VAL	2.5
1	P	374	CYS	2.5
1	B	35	SER	2.5
1	H	114	SER	2.5
1	A	359	GLU	2.5
1	G	166	GLU	2.5
1	B	311	ALA	2.5
1	B	316	HIS	2.5
1	M	280	HIS	2.5

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Mol	Chain	Res	Type	RSRZ
1	R	99	GLU	2.5
1	E	28	ALA	2.5
1	B	66	LYS	2.5
1	C	179	ASP	2.5
1	M	256	ASP	2.5
1	K	38	ASN	2.5
1	N	231	ASN	2.5
1	Q	232	ASN	2.5
1	A	162	ARG	2.5
1	A	296	THR	2.5
1	K	84	THR	2.5
1	K	341	THR	2.5
1	M	236	PHE	2.5
1	Q	296	THR	2.5
1	E	92	TYR	2.5
1	F	92	TYR	2.5
1	D	174	GLY	2.5
1	E	145	GLY	2.5
1	E	289	GLY	2.5
1	L	155	PRO	2.5
1	L	295	PRO	2.5
1	Q	334	GLY	2.5
1	M	166	GLU	2.5
1	C	282	LEU	2.5
1	F	212	LEU	2.5
1	R	257	LEU	2.5
1	B	218	CYS	2.5
1	J	47	LYS	2.5
1	E	29	ASP	2.5
1	F	160	ALA	2.5
1	N	28	ALA	2.5
1	A	263	ARG	2.5
1	H	384	ILE	2.5
1	Q	303	ARG	2.5
1	I	209	THR	2.4
1	K	63	THR	2.4
1	M	88	PHE	2.4
1	N	344	THR	2.4
1	B	161	GLU	2.4
1	C	279	GLY	2.4
1	D	91	GLU	2.4
1	D	281	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	K	334	GLY	2.4
1	N	48	GLU	2.4
1	A	75	PRO	2.4
1	I	80	TYR	2.4
1	O	345	TYR	2.4
1	B	258	LYS	2.4
1	K	390	LYS	2.4
1	N	377	LYS	2.4
1	B	274	LEU	2.4
1	B	356	SER	2.4
1	D	168	VAL	2.4
1	D	256	ASP	2.4
1	E	40	VAL	2.4
1	E	204	LEU	2.4
1	E	310	LEU	2.4
1	H	121	ASP	2.4
1	J	128	VAL	2.4
1	J	271	VAL	2.4
1	J	323	LEU	2.4
1	K	117	HIS	2.4
1	K	288	LEU	2.4
1	K	308	LEU	2.4
1	M	153	LEU	2.4
1	N	198	LEU	2.4
1	N	316	HIS	2.4
1	O	180	LEU	2.4
1	R	237	LEU	2.4
1	E	273	ARG	2.4
1	N	159	ARG	2.4
1	M	211	ALA	2.4
1	P	340	ALA	2.4
1	F	387	MET	2.4
1	Q	104	CYS	2.4
1	E	189	THR	2.4
1	G	130	GLY	2.4
1	J	85	GLY	2.4
1	L	23	GLY	2.4
1	O	101	PHE	2.4
1	B	118	PRO	2.4
1	J	120	PRO	2.4
1	B	185	TYR	2.4
1	H	80	TYR	2.4

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Mol	Chain	Res	Type	RSRZ
1	J	53	TYR	2.4
1	K	97	TYR	2.4
1	N	97	TYR	2.4
1	R	80	TYR	2.4
1	C	109	HIS	2.4
1	C	386	ASP	2.4
1	D	114	SER	2.4
1	J	65	ASP	2.4
1	K	102	ASP	2.4
1	A	257	LEU	2.4
1	A	361	VAL	2.4
1	B	133	GLU	2.4
1	B	169	VAL	2.4
1	H	128	VAL	2.4
1	I	302	VAL	2.4
1	J	306	VAL	2.4
1	J	360	LEU	2.4
1	R	323	LEU	2.4
1	N	91	GLU	2.4
1	R	314	GLU	2.4
1	B	156	ALA	2.4
1	D	167	LYS	2.4
1	F	66	LYS	2.4
1	H	119	ALA	2.4
1	J	373	ALA	2.4
1	K	258	LYS	2.4
1	L	82	LYS	2.4
1	M	160	ALA	2.4
1	E	382	GLN	2.4
1	G	240	ILE	2.4
1	G	384	ILE	2.4
1	O	142	ILE	2.4
1	O	228	ILE	2.4
1	G	294	CYS	2.4
1	J	227	GLY	2.4
1	L	389	PRO	2.4
1	M	113	PRO	2.4
1	Q	146	ARG	2.4
1	E	117	HIS	2.4
1	G	93	SER	2.4
1	P	170	SER	2.4
1	Q	250	SER	2.4

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Mol	Chain	Res	Type	RSRZ
1	I	185	TYR	2.4
1	J	97	TYR	2.4
1	P	357	GLU	2.4
1	D	274	LEU	2.4
1	G	355	LYS	2.4
1	K	193	LYS	2.4
1	N	126	LYS	2.4
1	O	323	LEU	2.4
1	Q	78	LYS	2.4
1	C	365	VAL	2.4
1	G	165	VAL	2.4
1	O	351	ALA	2.4
1	B	174	GLY	2.4
1	E	225	GLY	2.4
1	B	300	THR	2.4
1	H	46	THR	2.4
1	H	344	THR	2.4
1	N	246	ILE	2.4
1	D	21	GLU	2.4
1	L	59	PRO	2.4
1	M	346	ASP	2.4
1	Q	51	GLU	2.4
1	R	118	PRO	2.4
1	E	111	PHE	2.4
1	I	264	PHE	2.4
1	P	236	PHE	2.4
1	Q	264	PHE	2.4
1	R	111	PHE	2.4
1	E	77	ASN	2.4
1	G	369	ASN	2.4
1	N	30	ASN	2.4
1	D	50	TYR	2.4
1	J	49	LEU	2.4
1	N	339	LEU	2.4
1	C	259	ALA	2.4
1	C	381	GLY	2.4
1	D	380	ALA	2.4
1	G	157	MET	2.4
1	H	227	GLY	2.4
1	M	279	GLY	2.4
1	M	354	GLY	2.4
1	R	381	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	286	ASP	2.4
1	C	214	THR	2.4
1	G	167	LYS	2.4
1	I	63	THR	2.4
1	J	121	ASP	2.4
1	Q	179	ASP	2.4
1	K	108	ILE	2.4
1	P	384	ILE	2.4
1	H	239	TRP	2.4
1	J	12	ASN	2.4
1	J	350	TRP	2.4
1	C	136	TYR	2.4
1	A	370	LEU	2.4
1	B	257	LEU	2.4
1	D	268	LEU	2.4
1	K	133	GLU	2.4
1	B	178	GLY	2.4
1	F	151	VAL	2.4
1	G	182	GLY	2.4
1	I	137	VAL	2.4
1	I	361	VAL	2.4
1	L	129	GLY	2.4
1	M	57	VAL	2.4
1	N	103	LYS	2.4
1	O	151	VAL	2.4
1	O	322	MET	2.4
1	L	84	THR	2.4
1	B	249	ILE	2.4
1	L	232	ASN	2.4
1	M	108	ILE	2.4
1	R	250	SER	2.4
1	E	236	PHE	2.4
1	D	95	GLU	2.4
1	F	167	LYS	2.3
1	N	355	LYS	2.3
1	O	390	LYS	2.3
1	J	278	CYS	2.3
1	L	140	CYS	2.3
1	D	164	LEU	2.3
1	D	198	LEU	2.3
1	E	212	LEU	2.3
1	F	221	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	H	127	LEU	2.3
1	K	33	ASP	2.3
1	P	97	TYR	2.3
1	P	185	TYR	2.3
1	Q	94	TYR	2.3
1	P	225	GLY	2.3
1	J	148	VAL	2.3
1	K	368	VAL	2.3
1	L	361	VAL	2.3
1	N	160	ALA	2.3
1	I	232	ASN	2.3
1	M	38	ASN	2.3
1	B	188	THR	2.3
1	E	296	THR	2.3
1	F	113	PRO	2.3
1	N	389	PRO	2.3
1	O	155	PRO	2.3
1	F	142	ILE	2.3
1	L	108	ILE	2.3
1	O	372	ILE	2.3
1	A	83	LYS	2.3
1	R	11	LYS	2.3
1	P	31	PHE	2.3
1	L	350	TRP	2.3
1	B	55	ASP	2.3
1	E	121	ASP	2.3
1	F	174	GLY	2.3
1	J	279	GLY	2.3
1	O	61	GLY	2.3
1	O	335	GLY	2.3
1	R	281	GLY	2.3
1	A	288	LEU	2.3
1	B	50	TYR	2.3
1	J	274	LEU	2.3
1	A	301	VAL	2.3
1	E	191	ASN	2.3
1	O	371	LEU	2.3
1	A	380	ALA	2.3
1	C	28	ALA	2.3
1	E	363	VAL	2.3
1	G	238	VAL	2.3
1	K	271	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	P	72	VAL	2.3
1	P	248	VAL	2.3
1	Q	156	ALA	2.3
1	Q	160	ALA	2.3
1	B	250	SER	2.3
1	F	56	LYS	2.3
1	F	114	SER	2.3
1	F	154	PRO	2.3
1	G	120	PRO	2.3
1	I	258	LYS	2.3
1	L	138	LYS	2.3
1	L	162	ARG	2.3
1	L	215	THR	2.3
1	L	333	THR	2.3
1	M	143	ARG	2.3
1	M	163	ARG	2.3
1	M	327	ARG	2.3
1	N	139	SER	2.3
1	O	135	LYS	2.3
1	O	333	THR	2.3
1	Q	186	PRO	2.3
1	R	186	PRO	2.3
1	R	344	THR	2.3
1	N	68	ILE	2.3
1	B	73	ASP	2.3
1	B	134	ASP	2.3
1	D	179	ASP	2.3
1	G	319	PHE	2.3
1	K	64	PHE	2.3
1	R	194	ASP	2.3
1	B	76	GLY	2.3
1	F	254	GLY	2.3
1	M	89	GLY	2.3
1	C	38	ASN	2.3
1	D	192	GLU	2.3
1	G	38	ASN	2.3
1	J	191	ASN	2.3
1	K	74	ASN	2.3
1	O	252	GLN	2.3
1	B	310	LEU	2.3
1	C	127	LEU	2.3
1	F	80	TYR	2.3

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Mol	Chain	Res	Type	RSRZ
1	G	136	TYR	2.3
1	I	325	LYS	2.3
1	K	173	LEU	2.3
1	K	183	LYS	2.3
1	L	183	LYS	2.3
1	Q	83	LYS	2.3
1	Q	288	LEU	2.3
1	A	280	HIS	2.3
1	D	307	HIS	2.3
1	G	259	ALA	2.3
1	C	188	THR	2.3
1	D	344	THR	2.3
1	H	93	SER	2.3
1	J	262	SER	2.3
1	M	87	VAL	2.3
1	N	128	VAL	2.3
1	P	160	ALA	2.3
1	K	154	PRO	2.3
1	L	186	PRO	2.3
1	L	300	THR	2.3
1	O	188	THR	2.3
1	P	63	THR	2.3
1	R	75	PRO	2.3
1	R	292	CYS	2.3
1	D	29	ASP	2.3
1	E	194	ASP	2.3
1	I	256	ASP	2.3
1	J	320	ASP	2.3
1	K	142	ILE	2.3
1	L	388	ILE	2.3
1	M	123	ASP	2.3
1	O	244	ASP	2.3
1	I	166	GLU	2.3
1	B	88	PHE	2.3
1	D	197	GLN	2.3
1	E	100	PHE	2.3
1	E	235	ASN	2.3
1	H	24	LYS	2.3
1	N	38	ASN	2.3
1	Q	36	LYS	2.3
1	R	24	LYS	2.3
1	A	198	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	E	180	LEU	2.3
1	G	288	LEU	2.3
1	I	257	LEU	2.3
1	J	117	HIS	2.3
1	K	94	TYR	2.3
1	L	173	LEU	2.3
1	L	250	SER	2.3
1	L	288	LEU	2.3
1	N	356	SER	2.3
1	O	139	SER	2.3
1	O	360	LEU	2.3
1	N	363	VAL	2.3
1	O	40	VAL	2.3
1	O	172	ALA	2.3
1	P	27	ALA	2.3
1	Q	184	TYR	2.3
1	Q	262	SER	2.3
1	A	62	VAL	2.3
1	A	306	VAL	2.3
1	D	75	PRO	2.3
1	D	248	VAL	2.3
1	F	168	VAL	2.3
1	L	87	VAL	2.3
1	B	346	ASP	2.3
1	G	134	ASP	2.3
1	K	200	GLU	2.3
1	K	201	ASP	2.3
1	P	99	GLU	2.3
1	D	26	LYS	2.3
1	E	294	CYS	2.3
1	E	390	LYS	2.3
1	G	382	GLN	2.3
1	H	292	CYS	2.3
1	M	104	CYS	2.3
1	O	24	LYS	2.3
1	P	96	CYS	2.3
1	B	309	ARG	2.3
1	D	77	ASN	2.3
1	D	178	GLY	2.3
1	F	61	GLY	2.3
1	G	285	ASN	2.3
1	I	332	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	L	178	GLY	2.3
1	R	178	GLY	2.3
1	L	100	PHE	2.3
1	C	307	HIS	2.3
1	D	202	HIS	2.3
1	M	109	HIS	2.3
1	A	184	TYR	2.3
1	C	58	THR	2.3
1	E	42	ALA	2.3
1	D	377	LYS	2.3
1	F	185	TYR	2.3
1	F	219	ALA	2.3
1	G	63	THR	2.3
1	G	341	THR	2.3
1	H	42	ALA	2.3
1	H	180	LEU	2.3
1	I	229	TRP	2.3
1	K	34	LEU	2.3
1	L	379	GLU	2.3
1	P	49	LEU	2.3
1	P	351	ALA	2.3
1	R	212	LEU	2.3
1	I	168	VAL	2.3
1	F	195	GLN	2.3
1	I	387	MET	2.3
1	J	361	VAL	2.3
1	M	62	VAL	2.3
1	N	154	PRO	2.3
1	P	363	VAL	2.3
1	Q	190	MET	2.3
1	R	215	THR	2.3
1	K	358	ARG	2.3
1	L	273	ARG	2.3
1	A	267	GLY	2.3
1	B	130	GLY	2.3
1	C	388	ILE	2.3
1	H	279	GLY	2.3
1	K	199	ILE	2.3
1	K	241	ASN	2.3
1	L	125	ASN	2.3
1	N	267	GLY	2.3
1	N	281	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	O	105	ILE	2.3
1	R	297	ASN	2.3
1	E	218	CYS	2.3
1	H	67	CYS	2.3
1	J	67	CYS	2.3
1	J	140	CYS	2.3
1	M	96	CYS	2.3
1	H	261	PHE	2.3
1	C	107	GLU	2.3
1	J	245	HIS	2.3
1	Q	321	GLU	2.3
1	B	315	LYS	2.3
1	D	383	SER	2.3
1	F	377	LYS	2.3
1	G	390	LYS	2.3
1	M	207	LYS	2.3
1	N	11	LYS	2.3
1	R	26	LYS	2.3
1	F	65	ASP	2.3
1	J	134	ASP	2.3
1	Q	121	ASP	2.3
1	A	295	PRO	2.3
1	C	380	ALA	2.3
1	H	189	THR	2.3
1	H	296	THR	2.3
1	H	300	THR	2.3
1	I	153	LEU	2.3
1	J	187	LEU	2.3
1	O	160	ALA	2.3
1	O	389	PRO	2.3
1	P	176	LEU	2.3
1	R	351	ALA	2.3
1	B	275	MET	2.2
1	D	54	TRP	2.2
1	K	350	TRP	2.2
1	K	387	MET	2.2
1	N	238	VAL	2.2
1	P	283	MET	2.2
1	F	76	GLY	2.2
1	G	129	GLY	2.2
1	H	30	ASN	2.2
1	Q	255	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	R	232	ASN	2.2
1	P	108	ILE	2.2
1	R	384	ILE	2.2
1	I	47	LYS	2.2
1	K	234	LYS	2.2
1	O	26	LYS	2.2
1	D	280	HIS	2.2
1	C	140	CYS	2.2
1	F	17	SER	2.2
1	L	79	PHE	2.2
1	O	262	SER	2.2
1	R	236	PHE	2.2
1	R	252	GLN	2.2
1	I	309	ARG	2.2
1	K	113	PRO	2.2
1	A	308	LEU	2.2
1	B	49	LEU	2.2
1	B	288	LEU	2.2
1	D	288	LEU	2.2
1	F	213	LEU	2.2
1	G	188	THR	2.2
1	H	378	LEU	2.2
1	P	164	LEU	2.2
1	Q	214	THR	2.2
1	R	371	LEU	2.2
1	A	290	TYR	2.2
1	D	133	GLU	2.2
1	D	272	GLU	2.2
1	F	277	GLU	2.2
1	H	238	VAL	2.2
1	I	283	MET	2.2
1	K	190	MET	2.2
1	P	157	MET	2.2
1	H	277	GLU	2.2
1	O	225	GLY	2.2
1	R	53	TYR	2.2
1	F	126	LYS	2.2
1	A	202	HIS	2.2
1	N	105	ILE	2.2
1	R	249	ILE	2.2
1	Q	252	GLN	2.2
1	A	266	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	13	ARG	2.2
1	I	43	SER	2.2
1	J	250	SER	2.2
1	N	287	ARG	2.2
1	R	343	SER	2.2
1	J	261	PHE	2.2
1	O	88	PHE	2.2
1	B	67	CYS	2.2
1	A	235	ASN	2.2
1	F	39	ASN	2.2
1	G	389	PRO	2.2
1	J	336	GLU	2.2
1	G	160	ALA	2.2
1	G	325	LYS	2.2
1	G	373	ALA	2.2
1	H	181	ALA	2.2
1	K	219	ALA	2.2
1	L	122	LEU	2.2
1	N	340	ALA	2.2
1	A	130	GLY	2.2
1	H	89	GLY	2.2
1	M	175	GLY	2.2
1	O	274	LEU	2.2
1	P	237	LEU	2.2
1	I	190	MET	2.2
1	O	41	MET	2.2
1	P	345	TYR	2.2
1	R	345	TYR	2.2
1	B	239	TRP	2.2
1	C	350	TRP	2.2
1	D	20	TRP	2.2
1	D	284	HIS	2.2
1	H	13	ARG	2.2
1	K	307	HIS	2.2
1	L	16	HIS	2.2
1	L	375	ASP	2.2
1	P	121	ASP	2.2
1	C	348	SER	2.2
1	G	228	ILE	2.2
1	I	347	ILE	2.2
1	M	388	ILE	2.2
1	Q	338	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	F	99	GLU	2.2
1	O	79	PHE	2.2
1	P	78	LYS	2.2
1	A	191	ASN	2.2
1	F	125	ASN	2.2
1	F	232	ASN	2.2
1	M	155	PRO	2.2
1	B	215	THR	2.2
1	I	267	GLY	2.2
1	K	127	LEU	2.2
1	K	237	LEU	2.2
1	L	294	CYS	2.2
1	L	364	LEU	2.2
1	N	156	ALA	2.2
1	N	354	GLY	2.2
1	D	204	LEU	2.2
1	Q	259	ALA	2.2
1	R	282	LEU	2.2
1	E	298	MET	2.2
1	B	386	ASP	2.2
1	G	266	ARG	2.2
1	K	159	ARG	2.2
1	F	97	TYR	2.2
1	A	91	GLU	2.2
1	C	26	LYS	2.2
1	D	325	LYS	2.2
1	G	234	LYS	2.2
1	J	91	GLU	2.2
1	O	68	ILE	2.2
1	P	249	ILE	2.2
1	N	125	ASN	2.2
1	E	64	PHE	2.2
1	I	317	PRO	2.2
1	L	101	PHE	2.2
1	R	101	PHE	2.2
1	C	209	THR	2.2
1	I	178	GLY	2.2
1	P	175	GLY	2.2
1	P	381	GLY	2.2
1	Q	182	GLY	2.2
1	G	69	GLN	2.2
1	K	318	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	M	172	ALA	2.2
1	R	358	ARG	2.2
1	A	179	ASP	2.2
1	C	196	GLU	2.2
1	H	339	LEU	2.2
1	J	95	GLU	2.2
1	C	284	HIS	2.2
1	E	47	LYS	2.2
1	M	82	LYS	2.2
1	M	167	LYS	2.2
1	M	314	GLU	2.2
1	E	278	CYS	2.2
1	I	87	VAL	2.2
1	O	131	VAL	2.2
1	R	271	VAL	2.2
1	D	338	SER	2.2
1	K	114	SER	2.2
1	P	50	TYR	2.2
1	P	12	ASN	2.2
1	J	291	ILE	2.2
1	L	246	ILE	2.2
1	Q	372	ILE	2.2
1	B	229	TRP	2.2
1	D	229	TRP	2.2
1	B	255	GLY	2.2
1	D	358	ARG	2.2
1	H	182	GLY	2.2
1	J	118	PRO	2.2
1	K	279	GLY	2.2
1	M	76	GLY	2.2
1	K	359	GLU	2.2
1	L	261	PHE	2.2
1	N	79	PHE	2.2
1	O	309	ARG	2.2
1	C	200	GLU	2.2
1	Q	205	PHE	2.2
1	D	52	LYS	2.2
1	E	123	ASP	2.2
1	K	29	ASP	2.2
1	K	385	ASP	2.2
1	O	194	ASP	2.2
1	R	135	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	219	ALA	2.2
1	J	259	ALA	2.2
1	D	370	LEU	2.2
1	L	198	LEU	2.2
1	E	72	VAL	2.2
1	K	250	SER	2.2
1	N	14	VAL	2.2
1	O	93	SER	2.2
1	R	305	SER	2.2
1	A	86	CYS	2.2
1	H	235	ASN	2.2
1	I	191	ASN	2.2
1	N	218	CYS	2.2
1	O	96	CYS	2.2
1	C	273	ARG	2.1
1	D	48	GLU	2.1
1	F	270	GLU	2.1
1	H	95	GLU	2.1
1	I	220	ARG	2.1
1	K	372	ILE	2.1
1	L	195	GLN	2.1
1	L	358	ARG	2.1
1	N	228	ILE	2.1
1	O	388	ILE	2.1
1	P	309	ARG	2.1
1	A	324	GLY	2.1
1	A	329	GLY	2.1
1	H	255	GLY	2.1
1	J	89	GLY	2.1
1	K	145	GLY	2.1
1	L	19	PRO	2.1
1	L	120	PRO	2.1
1	Q	267	GLY	2.1
1	E	73	ASP	2.1
1	E	239	TRP	2.1
1	H	79	PHE	2.1
1	I	79	PHE	2.1
1	K	111	PHE	2.1
1	L	312	PHE	2.1
1	C	42	ALA	2.1
1	H	316	HIS	2.1
1	K	202	HIS	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	282	LEU	2.1
1	A	326	LEU	2.1
1	E	49	LEU	2.1
1	E	198	LEU	2.1
1	J	198	LEU	2.1
1	K	310	LEU	2.1
1	Q	257	LEU	2.1
1	C	338	SER	2.1
1	F	241	ASN	2.1
1	I	60	ASN	2.1
1	K	232	ASN	2.1
1	M	139	SER	2.1
1	A	52	LYS	2.1
1	J	169	VAL	2.1
1	K	168	VAL	2.1
1	C	318	ARG	2.1
1	E	263	ARG	2.1
1	K	69	GLN	2.1
1	Q	47	LYS	2.1
1	Q	163	ARG	2.1
1	D	55	ASP	2.1
1	D	228	ILE	2.1
1	E	90	ASP	2.1
1	I	171	ASP	2.1
1	J	102	ASP	2.1
1	L	90	ASP	2.1
1	M	182	GLY	2.1
1	M	217	GLY	2.1
1	M	218	CYS	2.1
1	P	347	ILE	2.1
1	Q	320	ASP	2.1
1	R	374	CYS	2.1
1	C	280	HIS	2.1
1	C	316	HIS	2.1
1	E	280	HIS	2.1
1	J	64	PHE	2.1
1	K	70	THR	2.1
1	K	101	PHE	2.1
1	K	124	HIS	2.1
1	N	63	THR	2.1
1	A	42	ALA	2.1
1	B	119	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	211	ALA	2.1
1	J	222	TRP	2.1
1	C	51	GLU	2.1
1	C	231	ASN	2.1
1	D	149	LYS	2.1
1	F	297	ASN	2.1
1	L	12	ASN	2.1
1	M	78	LYS	2.1
1	M	321	GLU	2.1
1	C	382	GLN	2.1
1	F	328	LEU	2.1
1	G	310	LEU	2.1
1	L	159	ARG	2.1
1	N	212	LEU	2.1
1	P	353	LEU	2.1
1	D	169	VAL	2.1
1	H	87	VAL	2.1
1	I	169	VAL	2.1
1	L	301	VAL	2.1
1	R	306	VAL	2.1
1	B	299	GLY	2.1
1	C	89	GLY	2.1
1	D	129	GLY	2.1
1	E	255	GLY	2.1
1	H	366	ASP	2.1
1	I	320	ASP	2.1
1	G	80	TYR	2.1
1	J	255	GLY	2.1
1	L	299	GLY	2.1
1	N	254	GLY	2.1
1	Q	342	ASP	2.1
1	B	384	ILE	2.1
1	F	32	PRO	2.1
1	L	68	ILE	2.1
1	B	24	LYS	2.1
1	G	138	LYS	2.1
1	J	124	HIS	2.1
1	J	341	THR	2.1
1	K	26	LYS	2.1
1	K	233	GLU	2.1
1	M	112	LYS	2.1
1	M	189	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	M	325	LYS	2.1
1	O	278	CYS	2.1
1	N	333	THR	2.1
1	P	189	THR	2.1
1	Q	192	GLU	2.1
1	Q	209	THR	2.1
1	J	327	ARG	2.1
1	F	181	ALA	2.1
1	K	119	ALA	2.1
1	M	30	ASN	2.1
1	N	369	ASN	2.1
1	B	350	TRP	2.1
1	P	222	TRP	2.1
1	C	275	MET	2.1
1	C	328	LEU	2.1
1	D	180	LEU	2.1
1	E	176	LEU	2.1
1	G	190	MET	2.1
1	N	322	MET	2.1
1	Q	275	MET	2.1
1	C	256	ASP	2.1
1	B	368	VAL	2.1
1	D	227	GLY	2.1
1	G	334	GLY	2.1
1	K	260	VAL	2.1
1	M	174	GLY	2.1
1	N	217	GLY	2.1
1	H	193	LYS	2.1
1	J	193	LYS	2.1
1	K	126	LYS	2.1
1	L	149	LYS	2.1
1	I	389	PRO	2.1
1	L	359	GLU	2.1
1	K	50	TYR	2.1
1	N	186	PRO	2.1
1	O	94	TYR	2.1
1	P	223	PRO	2.1
1	A	246	ILE	2.1
1	O	109	HIS	2.1
1	O	280	HIS	2.1
1	A	252	GLN	2.1
1	H	252	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
1	J	197	GLN	2.1
1	F	333	THR	2.1
1	G	77	ASN	2.1
1	K	231	ASN	2.1
1	O	125	ASN	2.1
1	A	305	SER	2.1
1	B	144	CYS	2.1
1	B	265	ALA	2.1
1	G	96	CYS	2.1
1	G	144	CYS	2.1
1	G	383	SER	2.1
1	H	86	CYS	2.1
1	H	265	ALA	2.1
1	H	351	ALA	2.1
1	J	144	CYS	2.1
1	L	236	PHE	2.1
1	L	17	SER	2.1
1	L	292	CYS	2.1
1	P	67	CYS	2.1
1	P	144	CYS	2.1
1	Q	31	PHE	2.1
1	P	265	ALA	2.1
1	Q	337	SER	2.1
1	C	375	ASP	2.1
1	D	328	LEU	2.1
1	A	167	LYS	2.1
1	A	183	LYS	2.1
1	A	350	TRP	2.1
1	C	48	GLU	2.1
1	C	112	LYS	2.1
1	F	222	TRP	2.1
1	H	269	LEU	2.1
1	I	34	LEU	2.1
1	J	283	MET	2.1
1	O	121	ASP	2.1
1	P	90	ASP	2.1
1	P	244	ASP	2.1
1	L	212	LEU	2.1
1	H	355	LYS	2.1
1	L	95	GLU	2.1
1	O	222	TRP	2.1
1	P	253	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	354	GLY	2.1
1	E	329	GLY	2.1
1	M	245	HIS	2.1
1	P	382	GLN	2.1
1	F	30	ASN	2.1
1	M	80	TYR	2.1
1	F	249	ILE	2.1
1	H	105	ILE	2.1
1	L	228	ILE	2.1
1	P	240	ILE	2.1
1	Q	240	ILE	2.1
1	B	341	THR	2.1
1	C	300	THR	2.1
1	G	296	THR	2.1
1	J	296	THR	2.1
1	M	43	SER	2.1
1	Q	43	SER	2.1
1	C	211	ALA	2.1
1	D	193	LYS	2.1
1	E	380	ALA	2.1
1	G	79	PHE	2.1
1	I	134	ASP	2.1
1	J	26	LYS	2.1
1	J	82	LYS	2.1
1	K	51	GLU	2.1
1	L	88	PHE	2.1
1	L	211	ALA	2.1
1	L	276	LYS	2.1
1	Q	355	LYS	2.1
1	R	181	ALA	2.1
1	R	207	LYS	2.1
1	R	342	ASP	2.1
1	E	144	CYS	2.1
1	A	212	LEU	2.1
1	B	322	MET	2.1
1	C	237	LEU	2.1
1	C	308	LEU	2.1
1	F	122	LEU	2.1
1	I	182	GLY	2.1
1	J	326	LEU	2.1
1	L	190	MET	2.1
1	M	225	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	M	299	GLY	2.1
1	N	251	MET	2.1
1	P	227	GLY	2.1
1	Q	157	MET	2.1
1	R	89	GLY	2.1
1	G	361	VAL	2.1
1	H	137	VAL	2.1
1	M	260	VAL	2.1
1	P	271	VAL	2.1
1	F	316	HIS	2.1
1	G	349	ASN	2.1
1	I	223	PRO	2.1
1	D	136	TYR	2.1
1	E	233	GLU	2.1
1	G	50	TYR	2.1
1	H	185	TYR	2.1
1	P	234	LYS	2.1
1	Q	376	LYS	2.1
1	R	36	LYS	2.1
1	Q	356	SER	2.1
1	C	132	PHE	2.1
1	K	79	PHE	2.1
1	M	380	ALA	2.1
1	R	380	ALA	2.1
1	E	81	GLY	2.0
1	H	129	GLY	2.0
1	H	287	ARG	2.0
1	O	195	GLN	2.0
1	D	45	LEU	2.0
1	F	34	LEU	2.0
1	C	104	CYS	2.0
1	F	292	CYS	2.0
1	K	67	CYS	2.0
1	B	77	ASN	2.0
1	G	316	HIS	2.0
1	B	208	PRO	2.0
1	D	232	ASN	2.0
1	I	241	ASN	2.0
1	J	307	HIS	2.0
1	E	95	GLU	2.0
1	E	183	LYS	2.0
1	E	277	GLU	2.0

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Mol	Chain	Res	Type	RSRZ
1	L	377	LYS	2.0
1	R	57	VAL	2.0
1	R	222	TRP	2.0
1	N	115	ASP	2.0
1	A	188	THR	2.0
1	B	184	TYR	2.0
1	C	53	TYR	2.0
1	C	215	THR	2.0
1	M	170	SER	2.0
1	O	43	SER	2.0
1	O	158	SER	2.0
1	O	214	THR	2.0
1	O	337	SER	2.0
1	Q	158	SER	2.0
1	E	388	ILE	2.0
1	J	199	ILE	2.0
1	K	185	TYR	2.0
1	N	247	ARG	2.0
1	R	184	TYR	2.0
1	A	381	GLY	2.0
1	F	28	ALA	2.0
1	F	299	GLY	2.0
1	G	203	PHE	2.0
1	G	311	ALA	2.0
1	I	351	ALA	2.0
1	J	130	GLY	2.0
1	Q	210	GLY	2.0
1	Q	329	GLY	2.0
1	R	130	GLY	2.0
1	H	377	LYS	2.0
1	L	321	GLU	2.0
1	L	325	LYS	2.0
1	N	133	GLU	2.0
1	P	251	MET	2.0
1	A	237	LEU	2.0
1	E	213	LEU	2.0
1	F	187	LEU	2.0
1	H	307	HIS	2.0
1	J	269	LEU	2.0
1	P	110	HIS	2.0
1	R	187	LEU	2.0
1	P	118	PRO	2.0

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Mol	Chain	Res	Type	RSRZ
1	G	221	ASP	2.0
1	J	375	ASP	2.0
1	L	152	CYS	2.0
1	N	365	VAL	2.0
1	A	247	ARG	2.0
1	C	239	TRP	2.0
1	D	263	ARG	2.0
1	E	266	ARG	2.0
1	H	222	TRP	2.0
1	O	170	SER	2.0
1	H	214	THR	2.0
1	N	252	GLN	2.0
1	Q	195	GLN	2.0
1	A	388	ILE	2.0
1	B	377	LYS	2.0
1	C	92	TYR	2.0
1	C	97	TYR	2.0
1	C	142	ILE	2.0
1	E	105	ILE	2.0
1	B	254	GLY	2.0
1	D	89	GLY	2.0
1	F	161	GLU	2.0
1	I	175	GLY	2.0
1	J	112	LYS	2.0
1	K	210	GLY	2.0
1	L	26	LYS	2.0
1	O	376	LYS	2.0
1	P	53	TYR	2.0
1	Q	50	TYR	2.0
1	R	98	LYS	2.0
1	J	351	ALA	2.0
1	Q	265	ALA	2.0
1	D	64	PHE	2.0
1	N	74	ASN	2.0
1	R	264	PHE	2.0
1	Q	245	HIS	2.0
1	C	371	LEU	2.0
1	G	323	LEU	2.0
1	G	371	LEU	2.0
1	I	198	LEU	2.0
1	J	176	LEU	2.0
1	P	123	ASP	2.0

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Mol	Chain	Res	Type	RSRZ
1	R	364	LEU	2.0
1	C	75	PRO	2.0
1	E	223	PRO	2.0
1	G	159	ARG	2.0
1	H	331	ARG	2.0
1	L	327	ARG	2.0
1	O	287	ARG	2.0
1	B	87	VAL	2.0
1	F	131	VAL	2.0
1	R	40	VAL	2.0
1	D	147	SER	2.0
1	E	149	LYS	2.0
1	M	52	LYS	2.0
1	P	337	SER	2.0
1	A	233	GLU	2.0
1	C	70	THR	2.0
1	K	270	GLU	2.0
1	M	51	GLU	2.0
1	Q	58	THR	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	NMG	D	504	8/8	0.44	6.96	20,23,24,24	0
4	MG	R	718	1/1	0.38	5.52	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	NMG	B	502	8/8	0.41	5.52	14,20,22,23	0
2	NMG	N	514	8/8	0.48	3.46	21,22,25,26	0
5	NO3	A	801	4/4	0.38	3.32	25,27,28,31	0
5	NO3	G	807	4/4	0.31	2.77	21,22,25,27	0
5	NO3	I	809	4/4	0.28	2.50	19,20,25,25	0
2	NMG	Q	517	8/8	0.45	2.44	25,28,33,33	0
5	NO3	J	810	4/4	0.35	2.44	22,24,25,29	0
4	MG	G	707	1/1	0.30	2.25	20,20,20,20	0
5	NO3	F	806	4/4	0.29	1.84	18,21,22,25	0
5	NO3	L	812	4/4	0.32	1.74	25,31,33,33	0
4	MG	M	713	1/1	0.29	1.66	9,9,9,9	0
5	NO3	D	804	4/4	0.28	1.12	21,23,23,27	0
2	NMG	F	506	8/8	0.28	1.04	16,19,24,24	0
4	MG	H	708	1/1	0.27	0.92	19,19,19,19	0
4	MG	N	714	1/1	0.28	0.61	22,22,22,22	0
4	MG	Q	717	1/1	0.27	0.44	12,12,12,12	0
2	NMG	G	507	8/8	0.28	0.44	20,23,25,25	0
2	NMG	E	505	8/8	0.27	0.27	25,28,29,31	0
4	MG	K	711	1/1	0.24	0.25	11,11,11,11	0
3	ADP	D	604	27/27	0.26	0.22	19,25,28,31	0
5	NO3	O	815	4/4	0.25	0.20	23,23,23,28	0
2	NMG	M	513	8/8	0.27	0.17	22,24,25,26	0
3	ADP	A	601	27/27	0.26	0.08	21,25,29,32	0
3	ADP	L	612	27/27	0.24	0.07	23,29,34,38	0
3	ADP	B	602	27/27	0.22	0.00	18,21,23,26	0
3	ADP	C	603	27/27	0.23	-0.02	13,20,22,24	0
2	NMG	K	511	8/8	0.25	-0.03	21,25,26,29	0
3	ADP	E	605	27/27	0.24	-0.04	19,25,29,31	0
2	NMG	I	509	8/8	0.23	-0.06	23,26,27,27	0
5	NO3	M	813	4/4	0.26	-0.10	21,22,24,24	0
5	NO3	K	811	4/4	0.21	-0.11	21,21,22,24	0
3	ADP	H	608	27/27	0.21	-0.32	14,17,21,23	0
3	ADP	M	613	27/27	0.23	-0.34	13,20,23,26	0
5	NO3	B	802	4/4	0.21	-0.37	20,21,24,24	0
3	ADP	J	610	27/27	0.21	-0.42	12,18,20,21	0
5	NO3	E	805	4/4	0.22	-0.45	24,25,26,29	0
2	NMG	O	515	8/8	0.21	-0.46	21,26,28,29	0
3	ADP	Q	617	27/27	0.26	-0.46	16,22,28,29	0
3	ADP	F	606	27/27	0.20	-0.47	13,18,22,24	0
3	ADP	I	609	27/27	0.22	-0.51	16,21,25,27	0
3	ADP	G	607	27/27	0.22	-0.51	21,27,29,30	0
5	NO3	C	803	4/4	0.20	-0.51	16,21,24,24	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	ADP	N	614	27/27	0.23	-0.52	10,20,23,26	0
3	ADP	O	615	27/27	0.23	-0.58	12,18,21,25	0
2	NMG	C	503	8/8	0.21	-0.61	16,22,25,25	0
4	MG	O	715	1/1	0.22	-0.62	10,10,10,10	0
3	ADP	P	616	27/27	0.22	-0.62	14,18,21,21	0
3	ADP	R	618	27/27	0.21	-0.64	13,17,21,23	0
5	NO3	N	814	4/4	0.23	-0.67	23,24,24,26	0
5	NO3	Q	817	4/4	0.24	-0.71	25,26,26,27	0
2	NMG	J	510	8/8	0.20	-0.76	25,26,28,29	0
5	NO3	P	816	4/4	0.22	-0.82	18,20,22,24	0
4	MG	C	703	1/1	0.20	-0.84	11,11,11,11	0
2	NMG	P	516	8/8	0.20	-0.87	15,17,20,24	0
3	ADP	K	611	27/27	0.19	-1.03	12,19,23,25	0
4	MG	P	716	1/1	0.22	-1.05	8,8,8,8	0
5	NO3	R	818	4/4	0.21	-1.16	14,19,22,22	0
2	NMG	L	512	8/8	0.18	-1.46	28,32,34,36	0
4	MG	J	710	1/1	0.20	-1.47	12,12,12,12	0
5	NO3	H	808	4/4	0.21	-1.49	20,21,22,23	0
2	NMG	H	508	8/8	0.17	-1.69	18,22,24,24	0
4	MG	L	712	1/1	0.20	-2.08	18,18,18,18	0
2	NMG	R	518	8/8	0.15	-2.37	15,17,22,23	0
4	MG	E	705	1/1	0.12	-2.41	14,14,14,14	0
2	NMG	A	501	8/8	0.17	-2.47	21,26,27,28	0
4	MG	A	701	1/1	0.15	-2.66	13,13,13,13	0
4	MG	F	706	1/1	0.18	-3.04	11,11,11,11	0
4	MG	D	704	1/1	0.11	-3.66	21,21,21,21	0
4	MG	I	709	1/1	0.16	-3.72	10,10,10,10	0
4	MG	B	702	1/1	0.10	-9.10	18,18,18,18	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.