



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 13, 2018 – 11:02 pm GMT

PDB ID : 5O7X
Title : CRYSTAL STRUCTURE OF S. CEREVISIAE CORE FACTOR AT 3.2A RESOLUTION
Authors : Engel, C.; Gubbey, T.; Neyer, S.; Sainsbury, S.; Oberthuer, C.; Baejen, C.; Bernecky, C.; Cramer, P.
Deposited on : 2017-06-09
Resolution : 3.20 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.3 (157068), CSD as539be (2018)
Xtriage (Phenix) : 1.13
EDS : trunk31020
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk31020

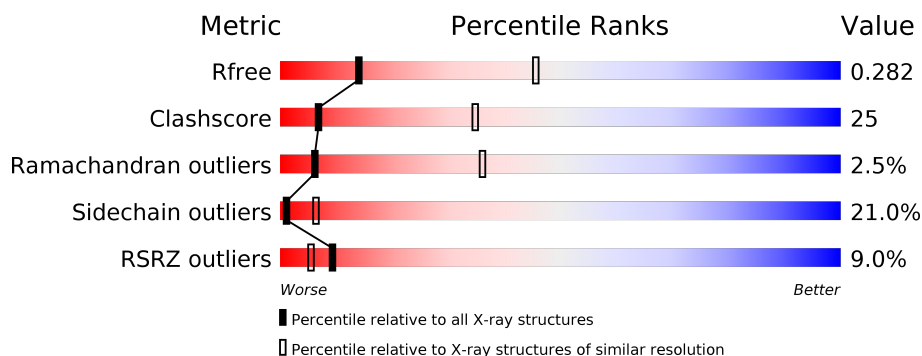
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	111664	1121 (3.22-3.18)
Clashscore	122126	1091 (3.20-3.20)
Ramachandran outliers	120053	1074 (3.20-3.20)
Sidechain outliers	120020	1073 (3.20-3.20)
RSRZ outliers	108989	1083 (3.22-3.18)

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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	894	<div> <div>7%</div> <div> <div></div> <div>30%</div> <div>27%</div> <div>9%</div> <div>•</div> <div>33%</div> </div> </div>
1	D	894	<div> <div>6%</div> <div> <div></div> <div>30%</div> <div>27%</div> <div>9%</div> <div>•</div> <div>33%</div> </div> </div>
1	G	894	<div> <div>7%</div> <div> <div></div> <div>30%</div> <div>27%</div> <div>9%</div> <div>•</div> <div>33%</div> </div> </div>
1	J	894	<div> <div>6%</div> <div> <div></div> <div>30%</div> <div>27%</div> <div>9%</div> <div>•</div> <div>33%</div> </div> </div>
1	M	894	<div> <div>6%</div> <div> <div></div> <div>30%</div> <div>27%</div> <div>9%</div> <div>•</div> <div>33%</div> </div> </div>
1	P	894	<div> <div>7%</div> <div> <div></div> <div>30%</div> <div>27%</div> <div>9%</div> <div>•</div> <div>33%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
2	B	514	
2	E	514	
2	H	514	
2	K	514	
2	N	514	
2	Q	514	
3	C	507	
3	F	507	
3	I	507	
3	L	507	
3	O	507	
3	R	507	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	SO4	A	1005	-	-	-	X
4	SO4	D	1004	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 63438 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called RNA polymerase I-specific transcription initiation factor RRN6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	598	Total	C	N	O	S	0	0	0
			4856	3092	824	929	11			
1	D	598	Total	C	N	O	S	0	0	0
			4856	3092	824	929	11			
1	G	598	Total	C	N	O	S	0	0	0
			4856	3092	824	929	11			
1	J	598	Total	C	N	O	S	0	0	0
			4856	3092	824	929	11			
1	M	598	Total	C	N	O	S	0	0	0
			4856	3092	824	929	11			
1	P	598	Total	C	N	O	S	0	0	0
			4856	3092	824	929	11			

- Molecule 2 is a protein called RNA polymerase I-specific transcription initiation factor RRN7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	377	Total	C	N	O	S	0	0	0
			3156	2055	526	559	16			
2	E	377	Total	C	N	O	S	0	0	0
			3156	2055	526	559	16			
2	H	377	Total	C	N	O	S	0	0	0
			3156	2055	526	559	16			
2	K	377	Total	C	N	O	S	0	0	0
			3156	2055	526	559	16			
2	N	377	Total	C	N	O	S	0	0	0
			3156	2055	526	559	16			
2	Q	377	Total	C	N	O	S	0	0	0
			3156	2055	526	559	16			

- Molecule 3 is a protein called RNA polymerase I-specific transcription initiation factor RRN11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	303	Total	C	N	O	S	0	0	0
			2535	1634	456	434	11			
3	F	303	Total	C	N	O	S	0	0	0
			2535	1634	456	434	11			
3	I	303	Total	C	N	O	S	0	0	0
			2535	1634	456	434	11			
3	L	303	Total	C	N	O	S	0	0	0
			2535	1634	456	434	11			
3	O	303	Total	C	N	O	S	0	0	0
			2535	1634	456	434	11			
3	R	303	Total	C	N	O	S	0	0	0
			2535	1634	456	434	11			

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	D	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		
4	F	1	Total	O	S	0	0
			5	4	1		
4	G	1	Total	O	S	0	0
			5	4	1		
4	G	1	Total	O	S	0	0
			5	4	1		
4	G	1	Total	O	S	0	0
			5	4	1		
4	H	1	Total	O	S	0	0
			5	4	1		
4	I	1	Total	O	S	0	0
			5	4	1		
4	J	1	Total	O	S	0	0
			5	4	1		
4	J	1	Total	O	S	0	0
			5	4	1		
4	J	1	Total	O	S	0	0
			5	4	1		
4	K	1	Total	O	S	0	0
			5	4	1		
4	L	1	Total	O	S	0	0
			5	4	1		
4	M	1	Total	O	S	0	0
			5	4	1		
4	M	1	Total	O	S	0	0
			5	4	1		
4	M	1	Total	O	S	0	0
			5	4	1		
4	M	1	Total	O	S	0	0
			5	4	1		
4	O	1	Total	O	S	0	0
			5	4	1		
4	P	1	Total	O	S	0	0
			5	4	1		
4	P	1	Total	O	S	0	0
			5	4	1		

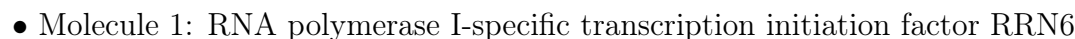
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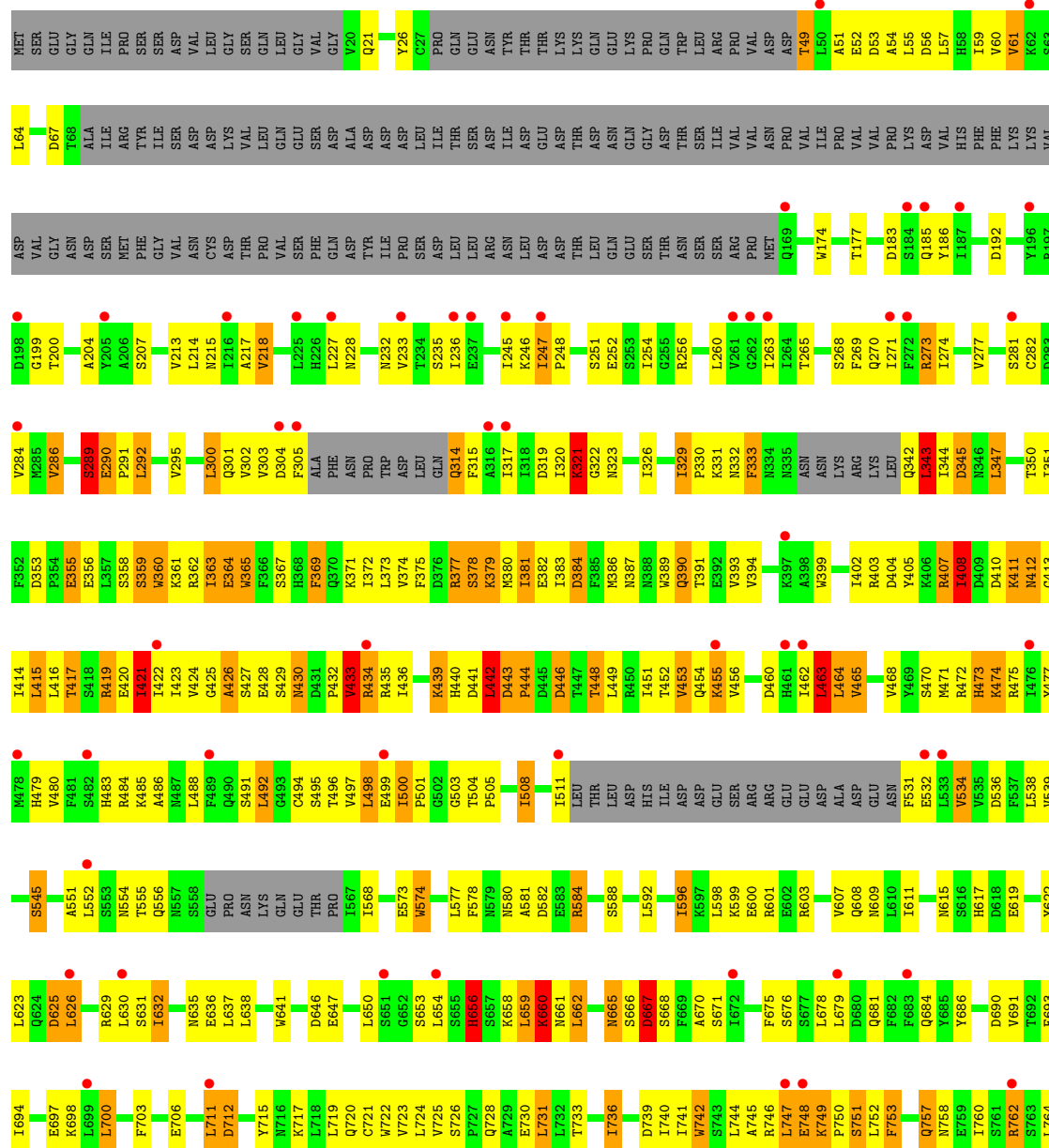
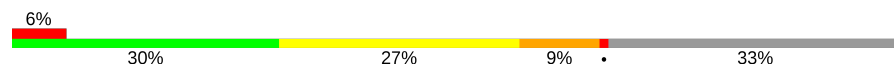
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	P	1	Total	O	S	0	0
			5	4	1		
4	P	1	Total	O	S	0	0
			5	4	1		
4	P	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

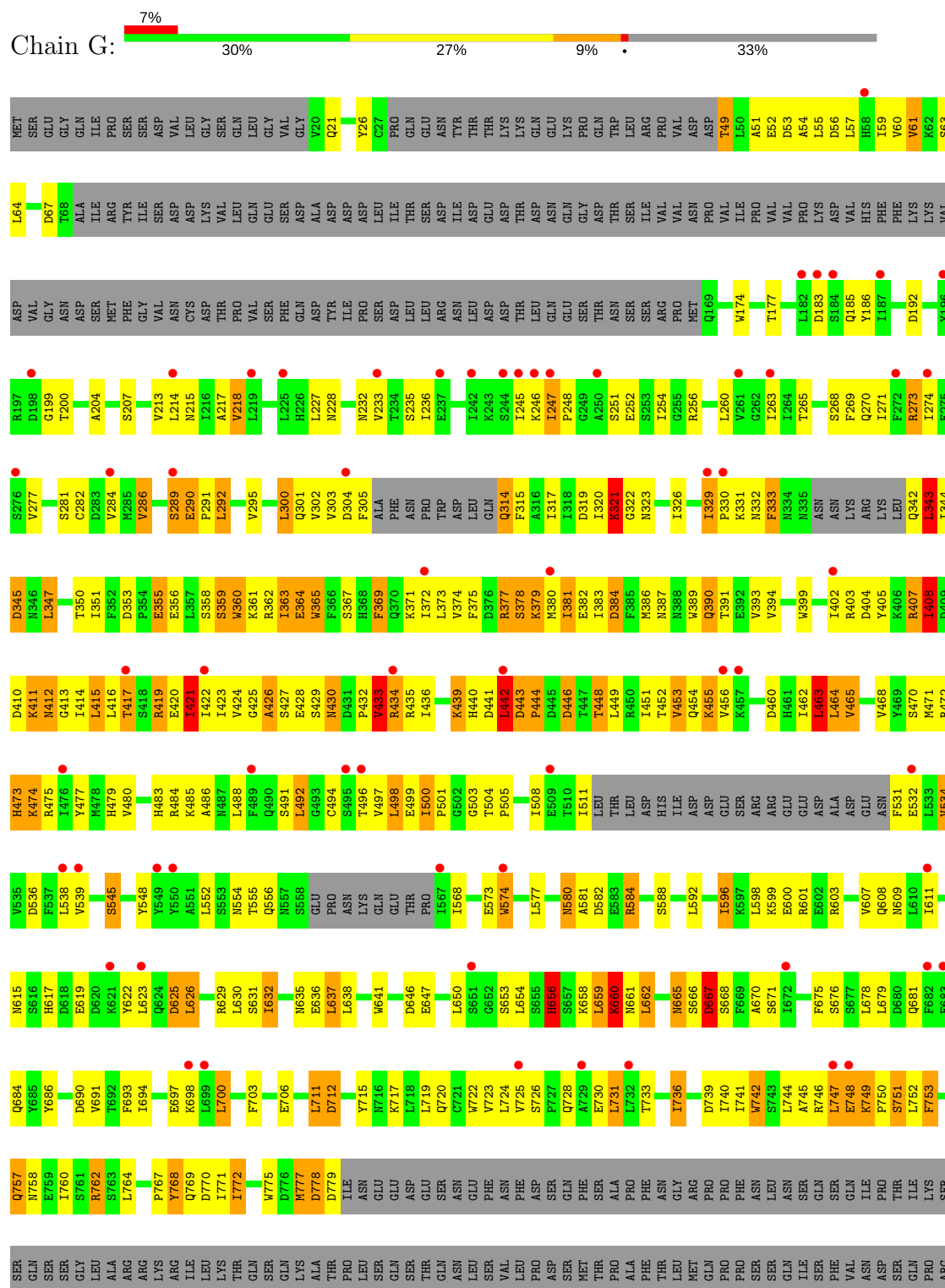
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	P	1	Total	Mg	0	0
			1	1		
5	G	1	Total	Mg	0	0
			1	1		
5	J	1	Total	Mg	0	0
			1	1		
5	D	1	Total	Mg	0	0
			1	1		
5	A	1	Total	Mg	0	0
			1	1		
5	M	1	Total	Mg	0	0
			1	1		



Chain D:



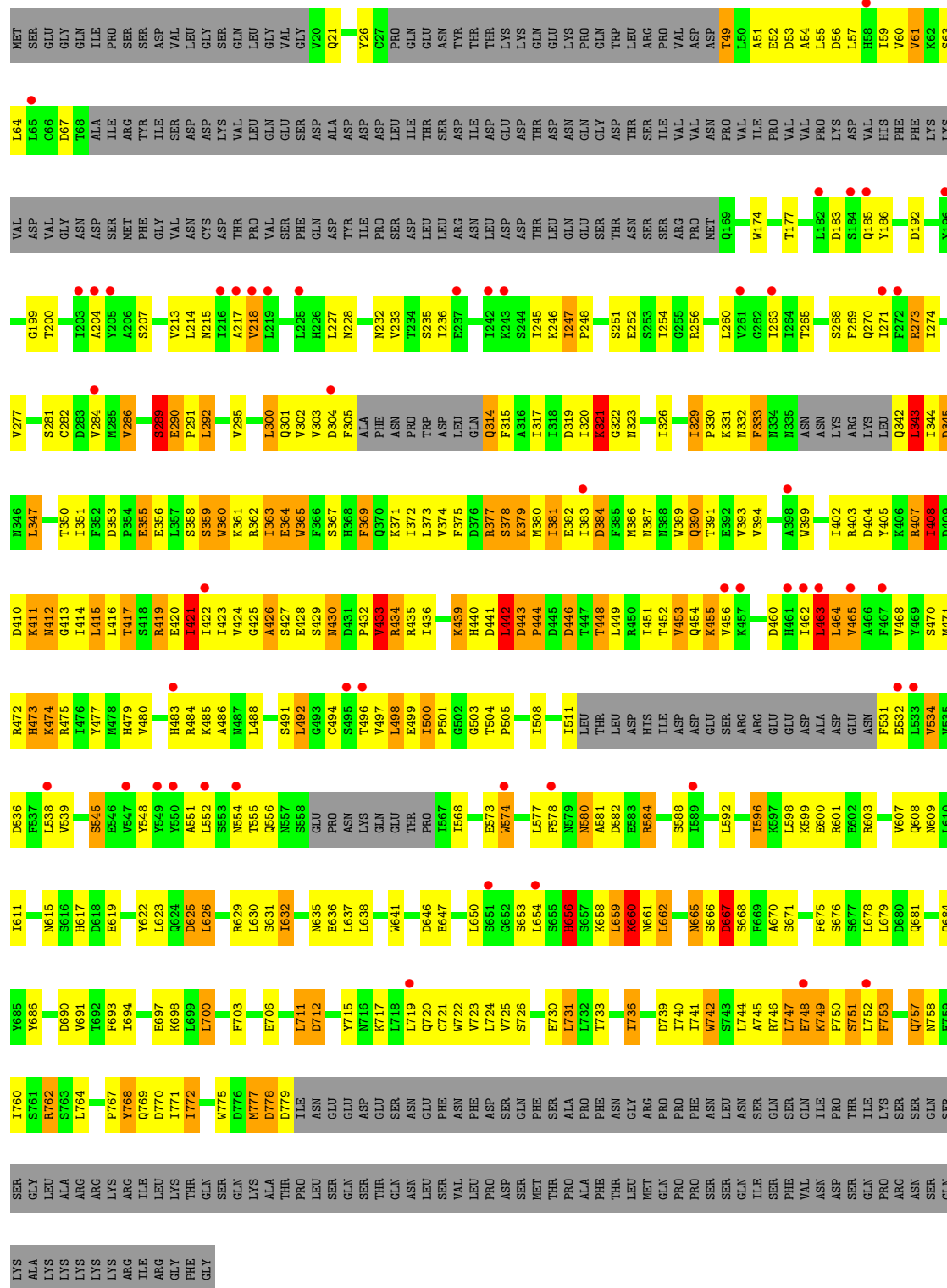
- Molecule 1: RNA polymerase I-specific transcription initiation factor RRN6



ASN
SER
GLN
LYS
LYS
ALA
LYS
LYS
LYS
LYS
ARG
ARG
ILE
GLY
PHE
GLY

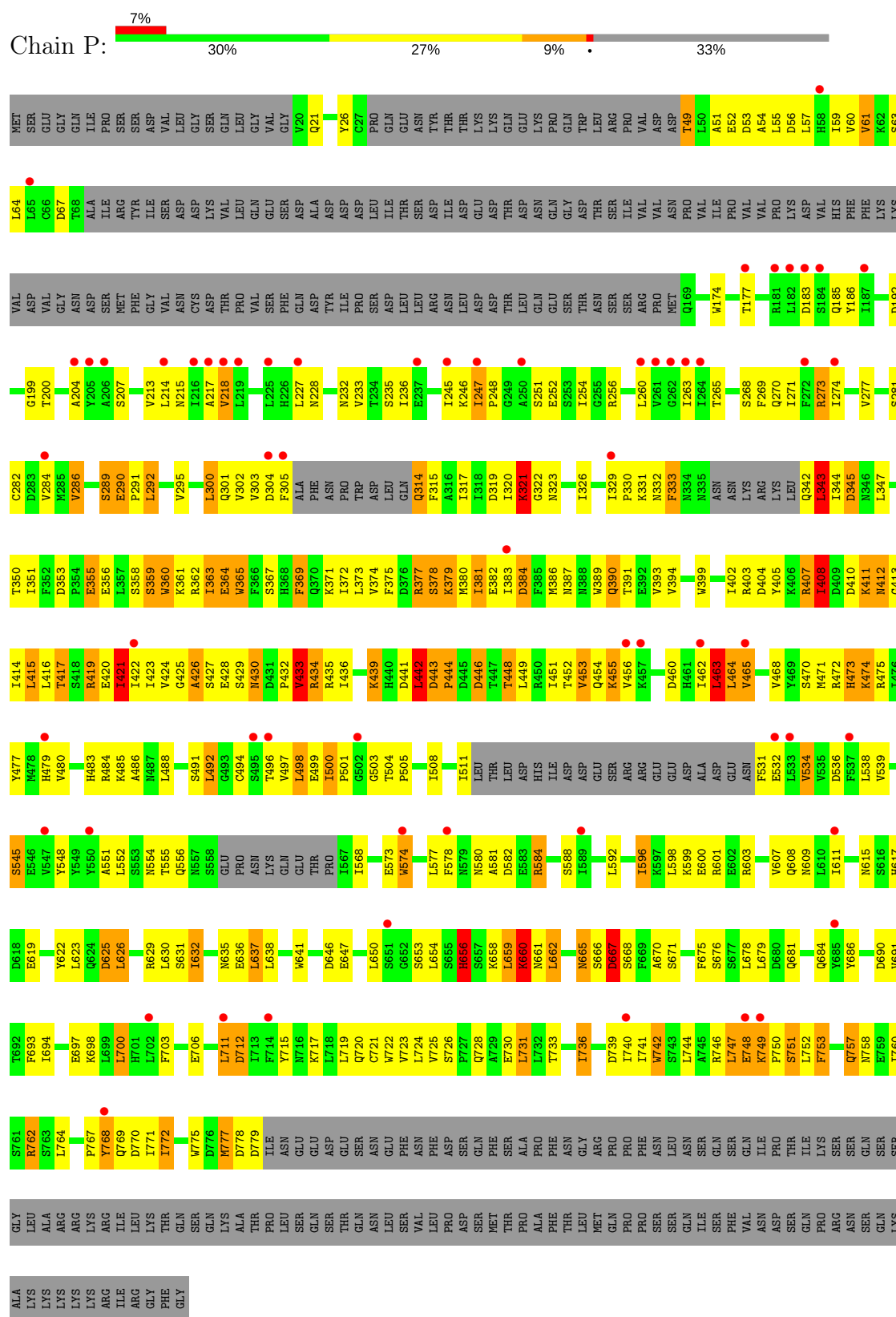
• Molecule 1: RNA polymerase I-specific transcription initiation factor RRN6

Chain J: 6% 30% 27% 9% 33%



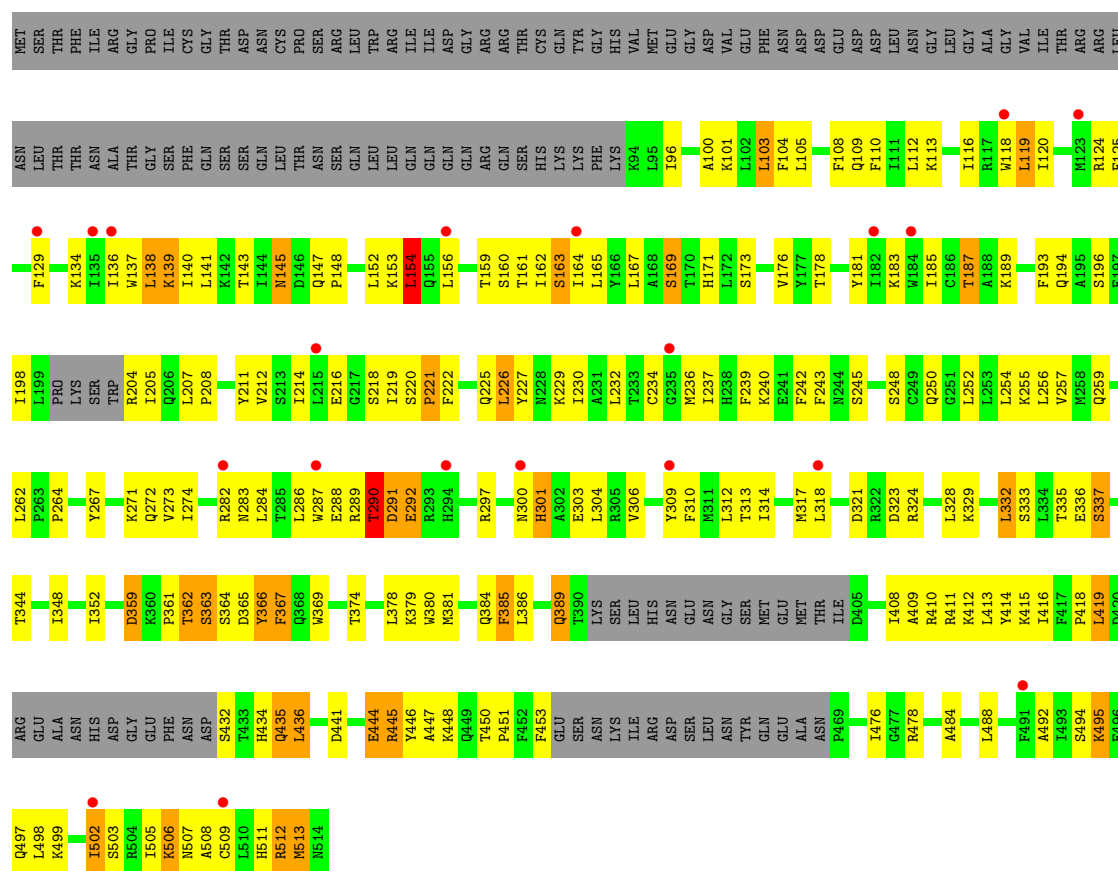
[illegible]

- Molecule 1: RNA polymerase I-specific transcription initiation factor RRN6

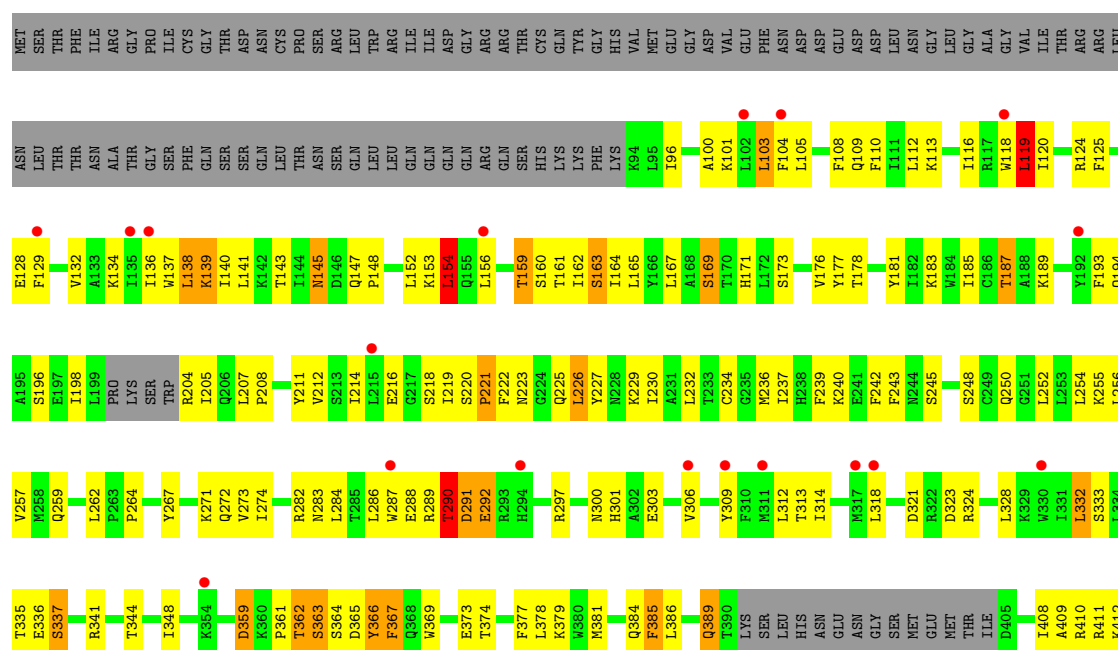


- Molecule 2: RNA polymerase I-specific transcription initiation factor RRN7

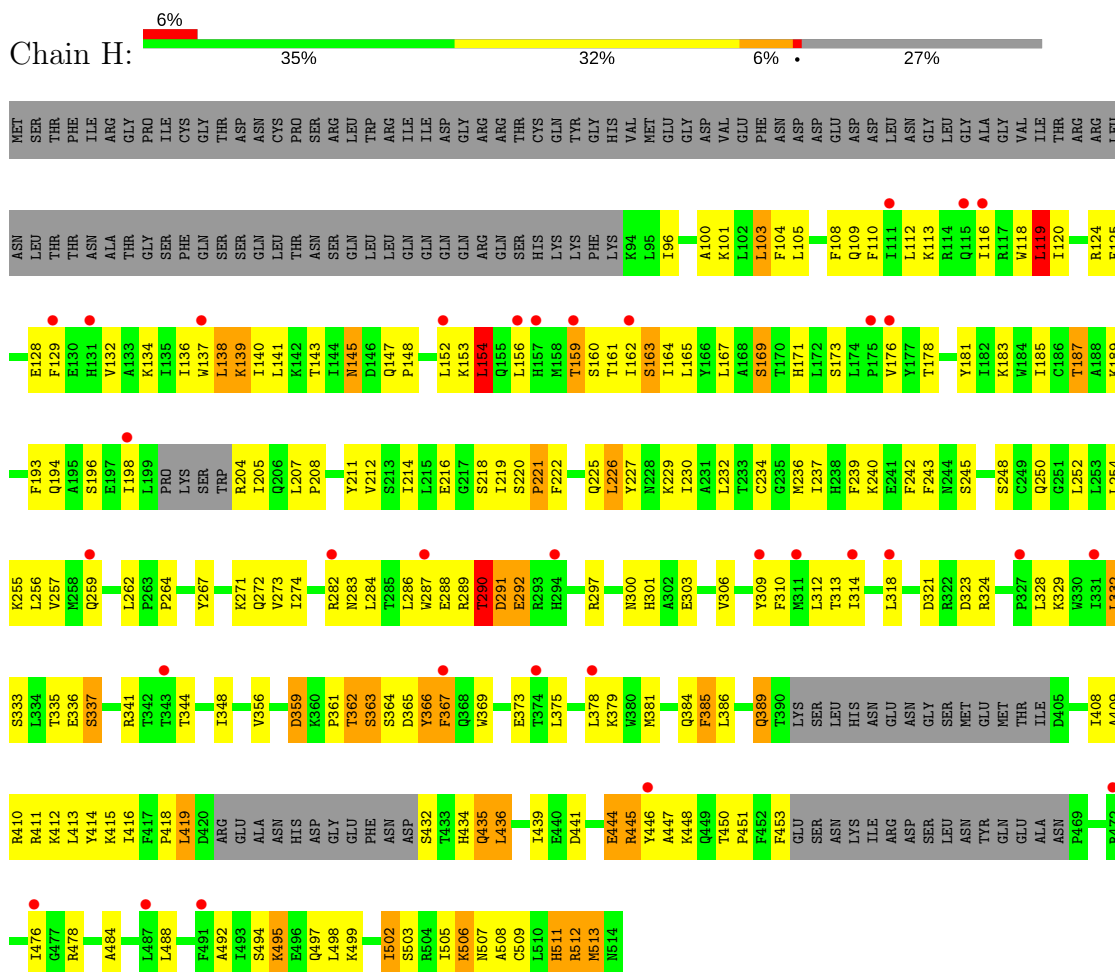




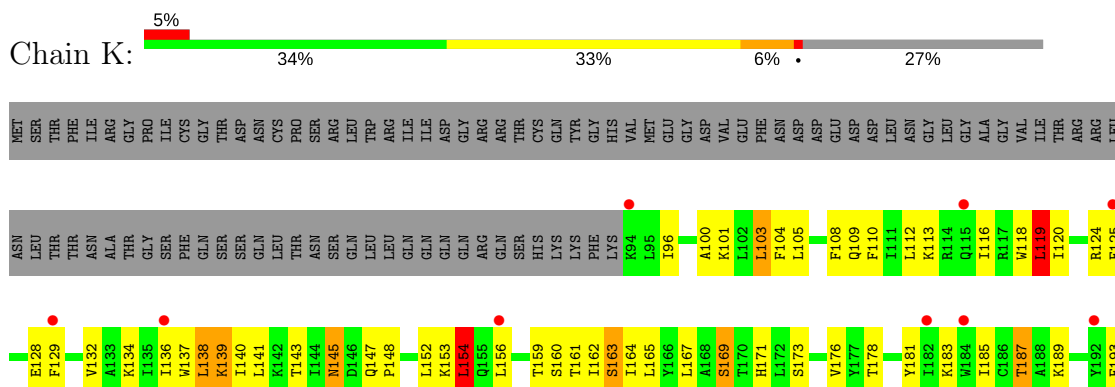
• Molecule 2: RNA polymerase I-specific transcription initiation factor RRN7

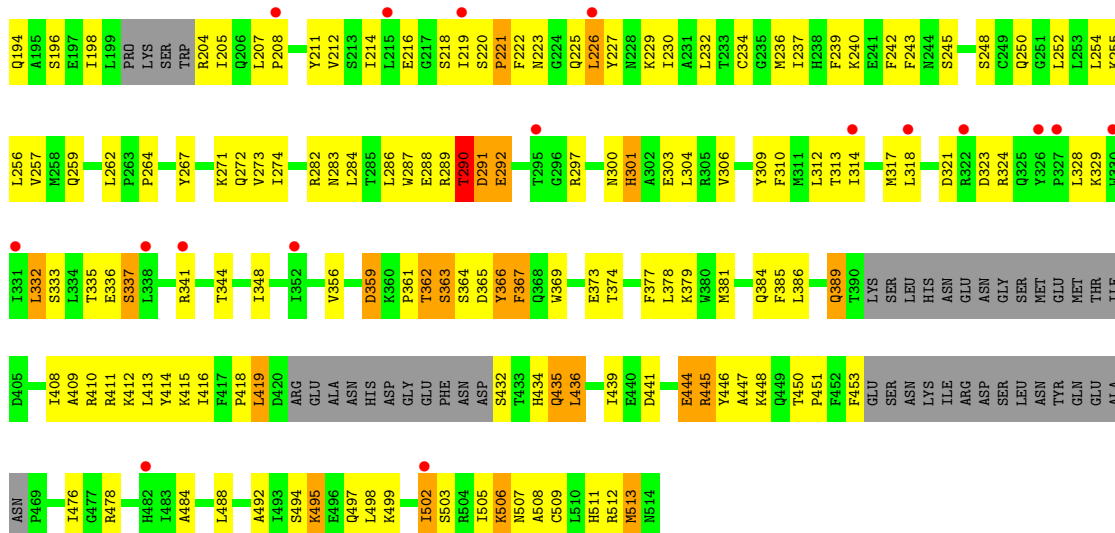


- Molecule 2: RNA polymerase I-specific transcription initiation factor RRN7

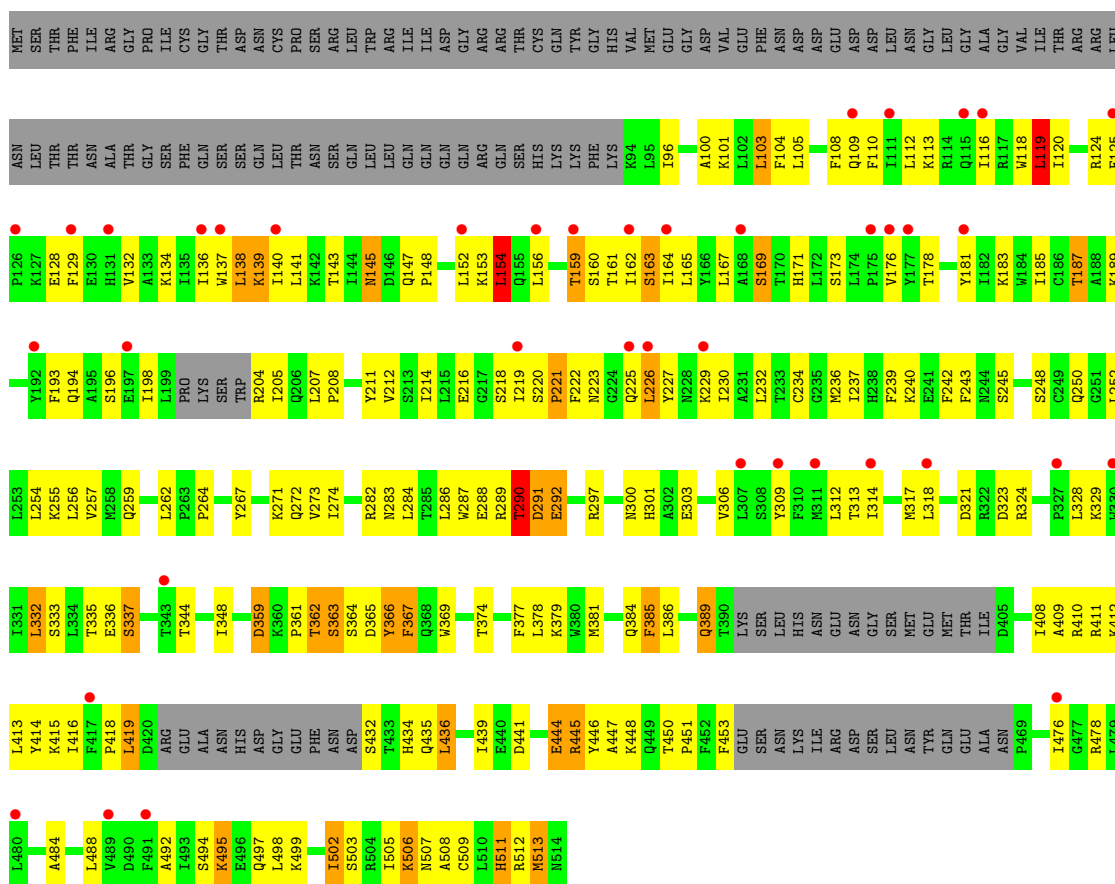


- Molecule 2: RNA polymerase I-specific transcription initiation factor RRN7



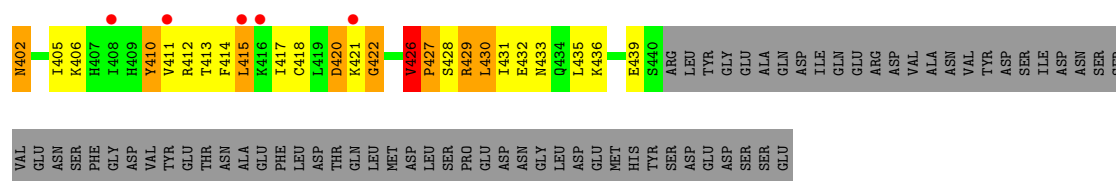


• Molecule 2: RNA polymerase I-specific transcription initiation factor RRN7

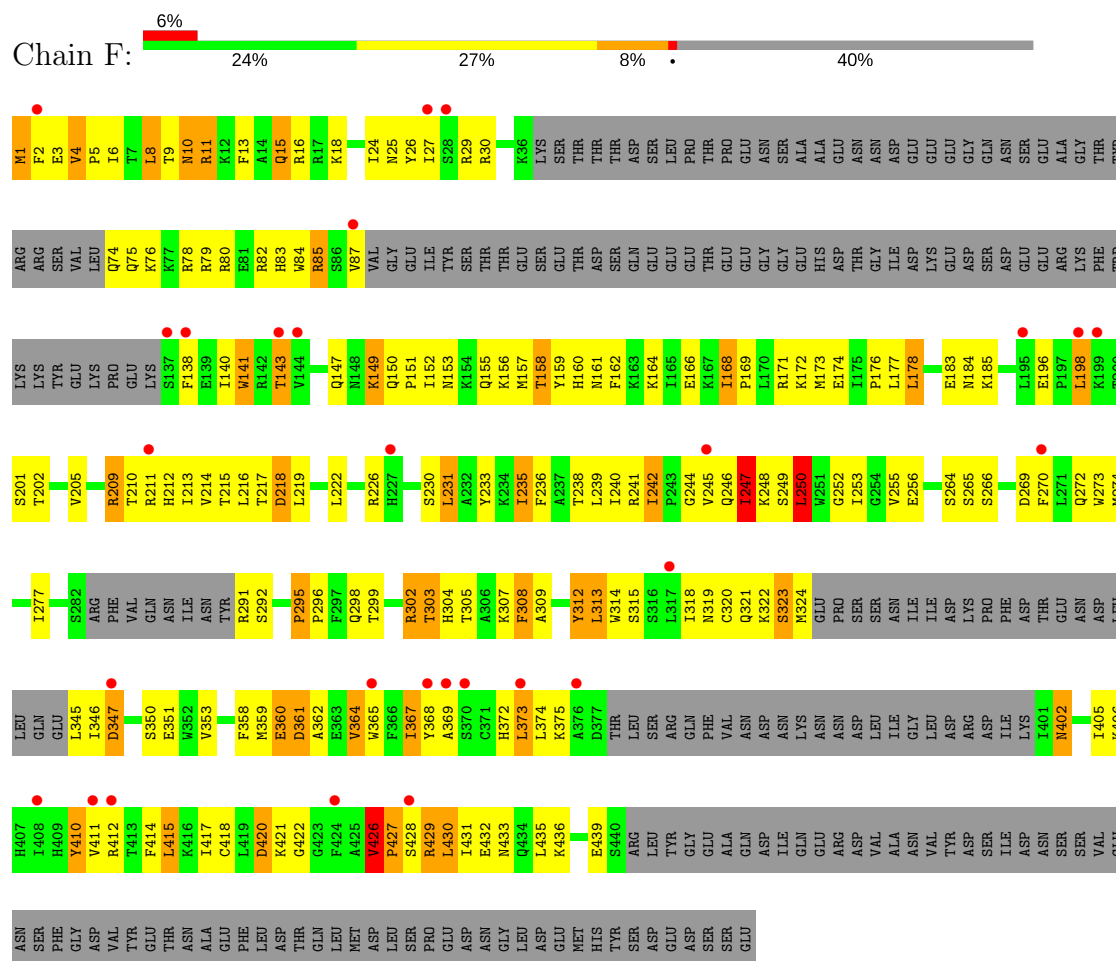


• Molecule 2: RNA polymerase I-specific transcription initiation factor RRN7

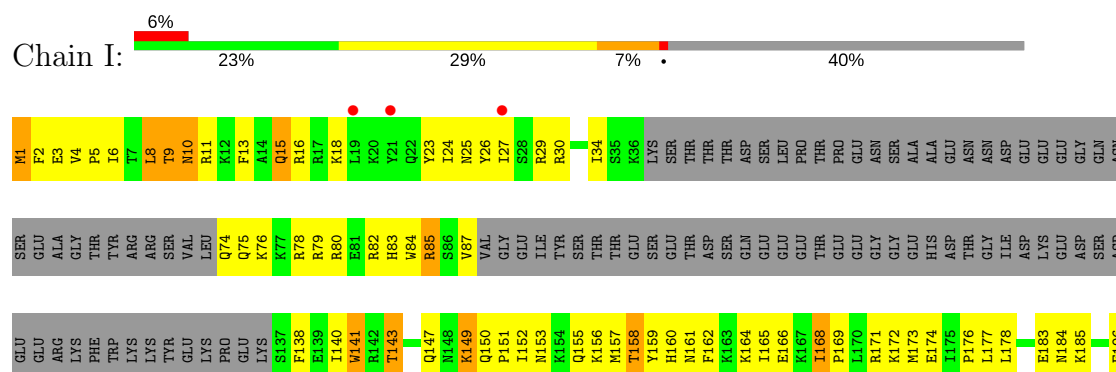


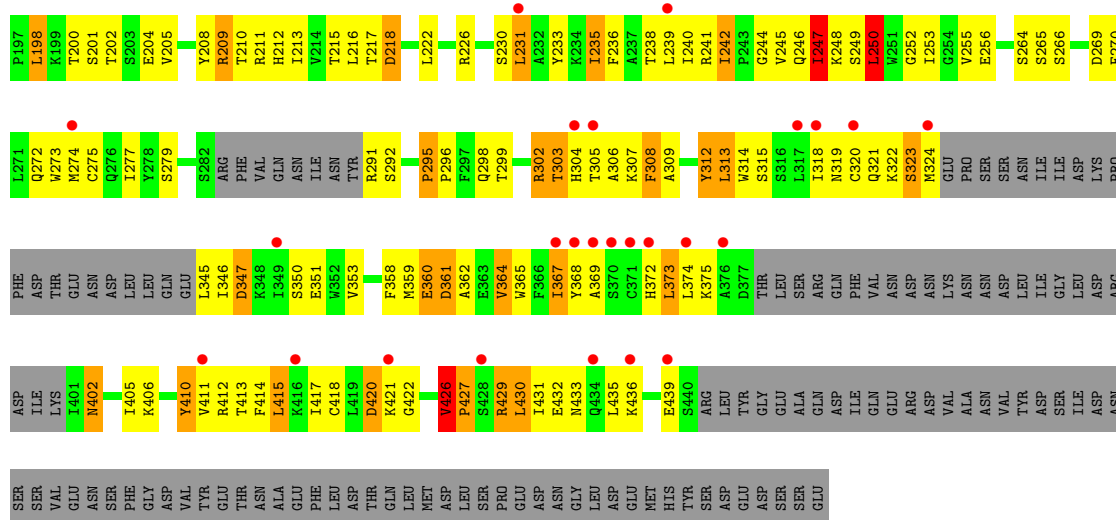


• Molecule 3: RNA polymerase I-specific transcription initiation factor RRN11

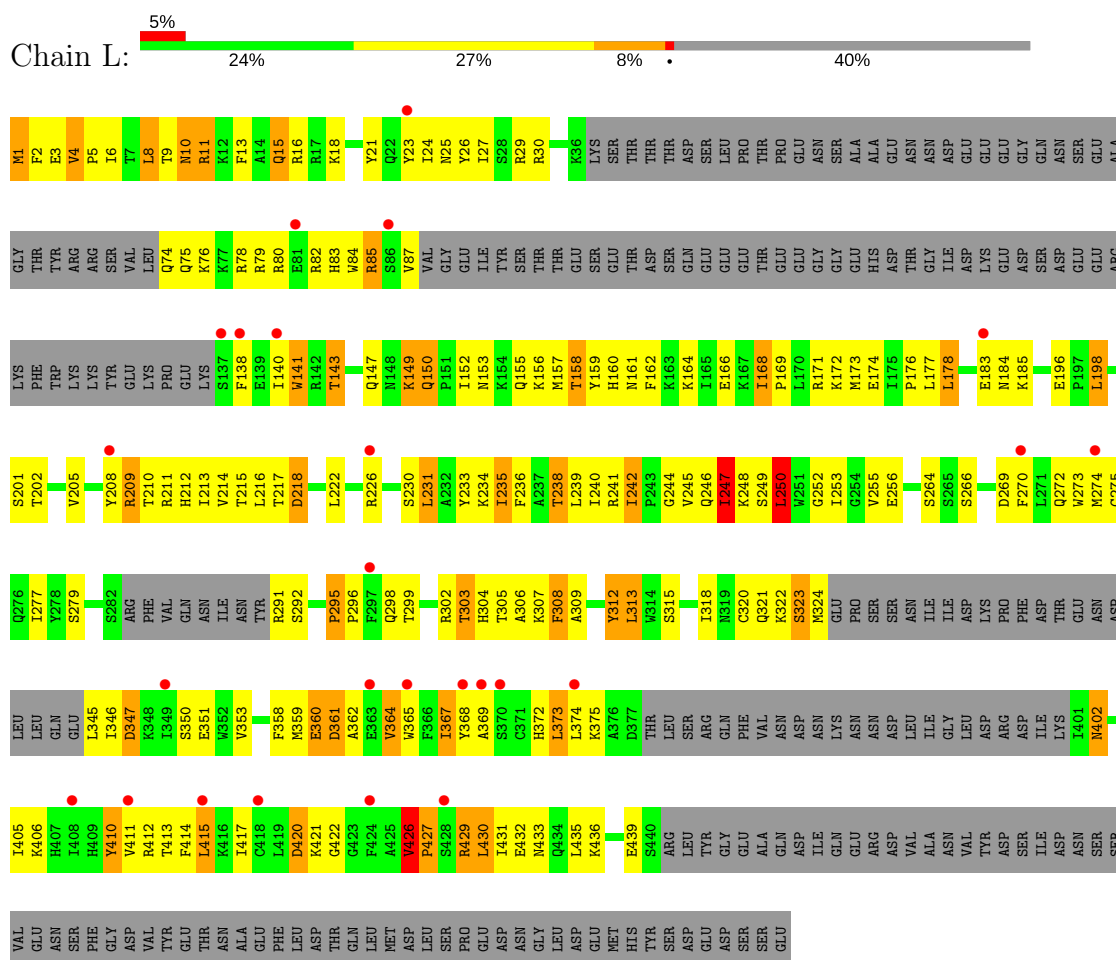


• Molecule 3: RNA polymerase I-specific transcription initiation factor RRN11

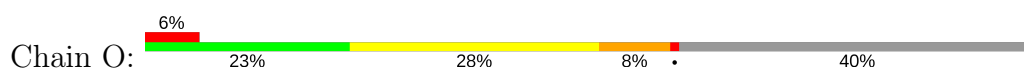


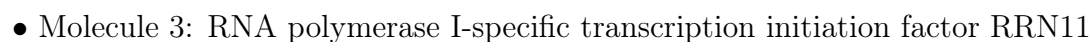


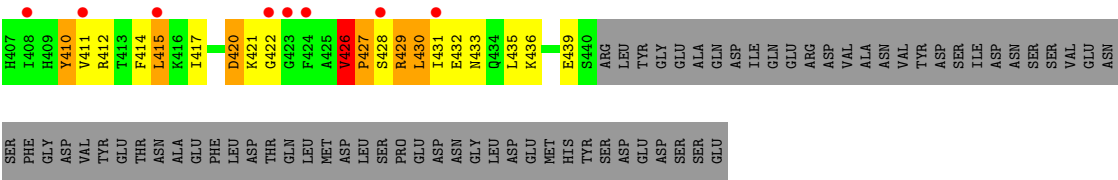
• Molecule 3: RNA polymerase I-specific transcription initiation factor RRN11



• Molecule 3: RNA polymerase I-specific transcription initiation factor RRN11







4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	109.07Å 109.14Å 385.64Å 90.02° 90.01° 59.98°	Depositor
Resolution (Å)	54.57 – 3.20 54.57 – 3.20	Depositor EDS
% Data completeness (in resolution range)	98.9 (54.57-3.20) 98.7 (54.57-3.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.40 (at 3.19Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
R, R_{free}	0.254 , 0.283 0.254 , 0.282	Depositor DCC
R_{free} test set	7461 reflections (2.97%)	wwPDB-VP
Wilson B-factor (Å ²)	127.2	Xtriage
Anisotropy	0.203	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 147.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.418 for k,-h+k,l 0.418 for h-k,h,l 0.410 for -h+k,-h,l 0.410 for -k,h-k,l 0.033 for h,h-k,-l 0.033 for -k,-h,-l 0.418 for -h,-k,l 0.033 for -h+k,k,-l 0.033 for h-k,-k,-l 0.033 for -h,-h+k,-l 0.034 for k,h,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	63438	wwPDB-VP
Average B, all atoms (Å ²)	149.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.42% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, SO4

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	0.40	0/4954	0.63	2/6707 (0.0%)
1	D	0.40	0/4954	0.63	2/6707 (0.0%)
1	G	0.40	0/4954	0.63	2/6707 (0.0%)
1	J	0.41	0/4954	0.63	2/6707 (0.0%)
1	M	0.40	0/4954	0.63	2/6707 (0.0%)
1	P	0.40	0/4954	0.63	2/6707 (0.0%)
2	B	0.37	0/3231	0.57	2/4362 (0.0%)
2	E	0.38	0/3231	0.57	2/4362 (0.0%)
2	H	0.38	0/3231	0.57	2/4362 (0.0%)
2	K	0.38	0/3231	0.57	2/4362 (0.0%)
2	N	0.38	0/3231	0.57	2/4362 (0.0%)
2	Q	0.37	0/3231	0.57	2/4362 (0.0%)
3	C	0.36	0/2592	0.57	2/3486 (0.1%)
3	F	0.36	0/2592	0.57	2/3486 (0.1%)
3	I	0.36	0/2592	0.57	1/3486 (0.0%)
3	L	0.36	0/2592	0.57	2/3486 (0.1%)
3	O	0.36	0/2592	0.57	1/3486 (0.0%)
3	R	0.36	0/2592	0.57	1/3486 (0.0%)
All	All	0.39	0/64662	0.60	33/87330 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	10
1	D	0	10
1	G	0	10
1	J	0	10
1	M	0	10

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	P	0	10
2	B	0	3
2	E	0	3
2	H	0	3
2	K	0	2
2	N	0	3
2	Q	0	3
3	C	0	4
3	F	0	4
3	I	0	4
3	L	0	3
3	O	0	4
3	R	0	4
All	All	0	100

There are no bond length outliers.

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	O	250	LEU	CA-CB-CG	8.02	133.75	115.30
3	L	250	LEU	CA-CB-CG	7.96	133.60	115.30
3	F	250	LEU	CA-CB-CG	7.88	133.44	115.30
3	R	250	LEU	CA-CB-CG	7.88	133.44	115.30
3	I	250	LEU	CA-CB-CG	7.85	133.35	115.30
3	C	250	LEU	CA-CB-CG	7.80	133.25	115.30
2	H	119	LEU	CA-CB-CG	6.74	130.80	115.30
2	N	119	LEU	CA-CB-CG	6.67	130.65	115.30
2	B	119	LEU	CA-CB-CG	6.66	130.61	115.30
2	K	119	LEU	CA-CB-CG	6.65	130.59	115.30
2	E	119	LEU	CA-CB-CG	6.64	130.57	115.30
2	Q	119	LEU	CA-CB-CG	6.62	130.53	115.30
1	P	463	LEU	CA-CB-CG	5.57	128.11	115.30
1	G	463	LEU	CA-CB-CG	5.56	128.09	115.30
1	J	463	LEU	CA-CB-CG	5.54	128.04	115.30
1	D	463	LEU	CA-CB-CG	5.54	128.04	115.30
1	M	463	LEU	CA-CB-CG	5.54	128.04	115.30
1	A	463	LEU	CA-CB-CG	5.52	127.99	115.30
1	D	343	LEU	CA-CB-CG	5.33	127.56	115.30
2	E	154	LEU	CA-CB-CG	5.33	127.55	115.30
2	K	154	LEU	CA-CB-CG	5.32	127.54	115.30
1	A	343	LEU	CA-CB-CG	5.31	127.51	115.30
2	B	154	LEU	CA-CB-CG	5.29	127.48	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	154	LEU	CA-CB-CG	5.29	127.47	115.30
1	P	343	LEU	CA-CB-CG	5.24	127.35	115.30
2	Q	154	LEU	CA-CB-CG	5.23	127.34	115.30
2	N	154	LEU	CA-CB-CG	5.22	127.31	115.30
1	M	343	LEU	CA-CB-CG	5.18	127.21	115.30
1	G	343	LEU	CA-CB-CG	5.17	127.19	115.30
1	J	343	LEU	CA-CB-CG	5.14	127.11	115.30
3	C	178	LEU	CA-CB-CG	5.09	127.01	115.30
3	F	178	LEU	CA-CB-CG	5.09	127.01	115.30
3	L	178	LEU	CA-CB-CG	5.02	126.85	115.30

There are no chirality outliers.

All (100) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	289	SER	Peptide
1	A	333	PHE	Peptide
1	A	365	TRP	Peptide
1	A	393	VAL	Peptide
1	A	408	ILE	Peptide
1	A	433	VAL	Peptide
1	A	442	LEU	Peptide
1	A	485	LYS	Peptide
1	A	500	ILE	Peptide
1	A	667	ASP	Peptide
2	B	221	PRO	Peptide
2	B	290	THR	Peptide
2	B	385	PHE	Peptide
3	C	247	ILE	Peptide
3	C	265	SER	Peptide
3	C	303	THR	Peptide
3	C	426	VAL	Peptide
1	D	289	SER	Peptide
1	D	333	PHE	Peptide
1	D	365	TRP	Peptide
1	D	393	VAL	Peptide
1	D	408	ILE	Peptide
1	D	433	VAL	Peptide
1	D	442	LEU	Peptide
1	D	485	LYS	Peptide
1	D	500	ILE	Peptide
1	D	667	ASP	Peptide

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Mol	Chain	Res	Type	Group
2	E	221	PRO	Peptide
2	E	290	THR	Peptide
2	E	385	PHE	Peptide
3	F	247	ILE	Peptide
3	F	265	SER	Peptide
3	F	303	THR	Peptide
3	F	426	VAL	Peptide
1	G	289	SER	Peptide
1	G	333	PHE	Peptide
1	G	365	TRP	Peptide
1	G	393	VAL	Peptide
1	G	408	ILE	Peptide
1	G	433	VAL	Peptide
1	G	442	LEU	Peptide
1	G	485	LYS	Peptide
1	G	500	ILE	Peptide
1	G	667	ASP	Peptide
2	H	221	PRO	Peptide
2	H	290	THR	Peptide
2	H	385	PHE	Peptide
3	I	247	ILE	Peptide
3	I	265	SER	Peptide
3	I	303	THR	Peptide
3	I	426	VAL	Peptide
1	J	289	SER	Peptide
1	J	333	PHE	Peptide
1	J	365	TRP	Peptide
1	J	393	VAL	Peptide
1	J	408	ILE	Peptide
1	J	433	VAL	Peptide
1	J	442	LEU	Peptide
1	J	485	LYS	Peptide
1	J	500	ILE	Peptide
1	J	667	ASP	Peptide
2	K	221	PRO	Peptide
2	K	290	THR	Peptide
3	L	247	ILE	Peptide
3	L	303	THR	Peptide
3	L	426	VAL	Peptide
1	M	289	SER	Peptide
1	M	333	PHE	Peptide
1	M	365	TRP	Peptide

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Mol	Chain	Res	Type	Group
1	M	393	VAL	Peptide
1	M	408	ILE	Peptide
1	M	433	VAL	Peptide
1	M	442	LEU	Peptide
1	M	485	LYS	Peptide
1	M	500	ILE	Peptide
1	M	667	ASP	Peptide
2	N	221	PRO	Peptide
2	N	290	THR	Peptide
2	N	385	PHE	Peptide
3	O	247	ILE	Peptide
3	O	265	SER	Peptide
3	O	303	THR	Peptide
3	O	426	VAL	Peptide
1	P	289	SER	Peptide
1	P	333	PHE	Peptide
1	P	365	TRP	Peptide
1	P	393	VAL	Peptide
1	P	408	ILE	Peptide
1	P	433	VAL	Peptide
1	P	442	LEU	Peptide
1	P	485	LYS	Peptide
1	P	500	ILE	Peptide
1	P	667	ASP	Peptide
2	Q	221	PRO	Peptide
2	Q	290	THR	Peptide
2	Q	385	PHE	Peptide
3	R	247	ILE	Peptide
3	R	265	SER	Peptide
3	R	303	THR	Peptide
3	R	426	VAL	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4856	0	4790	270	0
1	D	4856	0	4790	270	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	4856	0	4790	273	0
1	J	4856	0	4790	265	0
1	M	4856	0	4790	280	0
1	P	4856	0	4790	276	0
2	B	3156	0	3205	159	0
2	E	3156	0	3205	160	0
2	H	3156	0	3205	168	0
2	K	3156	0	3205	160	0
2	N	3156	0	3205	169	0
2	Q	3156	0	3205	166	0
3	C	2535	0	2609	134	0
3	F	2535	0	2609	130	0
3	I	2535	0	2609	134	0
3	L	2535	0	2609	129	0
3	O	2535	0	2609	136	0
3	R	2535	0	2609	129	0
4	A	25	0	0	1	0
4	D	20	0	0	1	0
4	F	5	0	0	0	0
4	G	15	0	0	1	0
4	H	5	0	0	0	0
4	I	5	0	0	0	0
4	J	15	0	0	1	0
4	K	5	0	0	0	0
4	L	5	0	0	0	0
4	M	20	0	0	1	0
4	O	5	0	0	0	0
4	P	25	0	0	1	0
5	A	1	0	0	0	0
5	D	1	0	0	0	0
5	G	1	0	0	0	0
5	J	1	0	0	0	0
5	M	1	0	0	0	0
5	P	1	0	0	0	0
All	All	63438	0	63624	3145	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 25.

All (3145) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:622:TYR:O	1:D:626:LEU:HB2	1.52	1.09
2:E:134:LYS:O	2:E:138:LEU:HB2	1.54	1.08
2:H:134:LYS:O	2:H:138:LEU:HB2	1.54	1.08
1:G:622:TYR:O	1:G:626:LEU:HB2	1.53	1.07
1:J:622:TYR:O	1:J:626:LEU:HB2	1.53	1.07
2:K:134:LYS:O	2:K:138:LEU:HB2	1.53	1.07
2:N:134:LYS:O	2:N:138:LEU:HB2	1.54	1.06
2:B:134:LYS:O	2:B:138:LEU:HB2	1.54	1.06
1:P:622:TYR:O	1:P:626:LEU:HB2	1.53	1.06
2:Q:134:LYS:O	2:Q:138:LEU:HB2	1.53	1.06
1:A:622:TYR:O	1:A:626:LEU:HB2	1.53	1.05
1:M:622:TYR:O	1:M:626:LEU:HB2	1.53	1.05
3:F:429:ARG:O	3:F:433:ASN:HB2	1.64	0.98
3:O:429:ARG:O	3:O:433:ASN:HB2	1.63	0.98
3:R:429:ARG:O	3:R:433:ASN:HB2	1.64	0.97
3:I:429:ARG:O	3:I:433:ASN:HB2	1.64	0.97
3:C:429:ARG:O	3:C:433:ASN:HB2	1.64	0.95
3:L:429:ARG:O	3:L:433:ASN:HB2	1.64	0.95
2:H:409:ALA:O	2:H:413:LEU:HB2	1.70	0.92
2:N:409:ALA:O	2:N:413:LEU:HB2	1.70	0.92
2:Q:409:ALA:O	2:Q:413:LEU:HB2	1.71	0.91
2:K:409:ALA:O	2:K:413:LEU:HB2	1.70	0.91
2:E:409:ALA:O	2:E:413:LEU:HB2	1.70	0.90
2:B:409:ALA:O	2:B:413:LEU:HB2	1.71	0.90
1:D:405:TYR:HE1	1:D:414:ILE:HG23	1.38	0.88
1:P:405:TYR:HE1	1:P:414:ILE:HG23	1.39	0.88
1:M:405:TYR:HE1	1:M:414:ILE:HG23	1.38	0.88
1:A:405:TYR:HE1	1:A:414:ILE:HG23	1.38	0.87
1:G:405:TYR:HE1	1:G:414:ILE:HG23	1.38	0.87
3:O:168:ILE:HG23	3:O:169:PRO:HD3	1.57	0.86
3:F:168:ILE:HG23	3:F:169:PRO:HD3	1.58	0.86
3:L:362:ALA:HB2	3:L:421:LYS:HB3	1.58	0.86
3:C:362:ALA:HB2	3:C:421:LYS:HB3	1.58	0.86
1:J:405:TYR:HE1	1:J:414:ILE:HG23	1.38	0.86
3:I:362:ALA:HB2	3:I:421:LYS:HB3	1.58	0.86
1:M:479:HIS:HE2	1:M:491:SER:HG	1.19	0.85
3:R:168:ILE:HG23	3:R:169:PRO:HD3	1.58	0.85
1:A:321:LYS:H	1:A:321:LYS:HD3	1.42	0.85
3:C:168:ILE:HG23	3:C:169:PRO:HD3	1.57	0.85
1:J:321:LYS:H	1:J:321:LYS:HD3	1.42	0.84
3:F:362:ALA:HB2	3:F:421:LYS:HB3	1.58	0.84
3:O:362:ALA:HB2	3:O:421:LYS:HB3	1.58	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:R:362:ALA:HB2	3:R:421:LYS:HB3	1.58	0.83
3:I:168:ILE:HG23	3:I:169:PRO:HD3	1.59	0.83
3:L:168:ILE:HG23	3:L:169:PRO:HD3	1.59	0.83
1:D:321:LYS:H	1:D:321:LYS:HD3	1.40	0.83
1:D:694:ILE:HB	1:D:746:ARG:HD3	1.61	0.83
1:G:321:LYS:HD3	1:G:321:LYS:H	1.42	0.82
1:G:694:ILE:HB	1:G:746:ARG:HD3	1.61	0.82
1:P:694:ILE:HB	1:P:746:ARG:HD3	1.61	0.82
1:J:694:ILE:HB	1:J:746:ARG:HD3	1.61	0.82
1:M:694:ILE:HB	1:M:746:ARG:HD3	1.61	0.81
1:P:321:LYS:HD3	1:P:321:LYS:H	1.43	0.81
1:D:658:LYS:HB3	1:D:660:LYS:H	1.45	0.81
1:P:658:LYS:HB3	1:P:660:LYS:H	1.45	0.81
1:A:694:ILE:HB	1:A:746:ARG:HD3	1.61	0.81
1:P:480:VAL:HB	1:P:492:LEU:HD21	1.64	0.80
1:M:321:LYS:HD3	1:M:321:LYS:H	1.46	0.80
2:Q:101:LYS:HG2	2:Q:152:LEU:HD11	1.63	0.80
2:H:101:LYS:HG2	2:H:152:LEU:HD11	1.63	0.80
1:M:658:LYS:HB3	1:M:660:LYS:H	1.46	0.80
1:A:480:VAL:HB	1:A:492:LEU:HD21	1.64	0.80
1:A:658:LYS:HB3	1:A:660:LYS:H	1.45	0.80
1:G:658:LYS:HB3	1:G:660:LYS:H	1.46	0.79
1:J:480:VAL:HB	1:J:492:LEU:HD21	1.64	0.79
1:D:480:VAL:HB	1:D:492:LEU:HD21	1.64	0.79
2:K:101:LYS:HG2	2:K:152:LEU:HD11	1.64	0.79
1:J:658:LYS:HB3	1:J:660:LYS:H	1.46	0.79
1:G:480:VAL:HB	1:G:492:LEU:HD21	1.64	0.79
3:L:432:GLU:O	3:L:435:LEU:N	2.17	0.78
3:I:432:GLU:O	3:I:435:LEU:N	2.16	0.78
1:M:480:VAL:HB	1:M:492:LEU:HD21	1.65	0.78
3:R:432:GLU:O	3:R:435:LEU:N	2.17	0.78
3:C:432:GLU:O	3:C:435:LEU:N	2.17	0.78
3:O:432:GLU:O	3:O:435:LEU:N	2.16	0.78
2:B:101:LYS:HG2	2:B:152:LEU:HD11	1.64	0.78
2:E:101:LYS:HG2	2:E:152:LEU:HD11	1.64	0.78
2:N:101:LYS:HG2	2:N:152:LEU:HD11	1.64	0.77
2:B:410:ARG:HA	2:B:413:LEU:HB3	1.66	0.77
1:D:598:LEU:HD23	1:D:601:ARG:HD2	1.65	0.77
2:K:410:ARG:HA	2:K:413:LEU:HB3	1.66	0.77
1:P:436:ILE:HD12	3:R:143:THR:HG23	1.66	0.77
1:J:598:LEU:HD23	1:J:601:ARG:HD2	1.65	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:432:GLU:O	3:F:435:LEU:N	2.16	0.77
2:H:410:ARG:HA	2:H:413:LEU:HB3	1.66	0.77
3:L:6:ILE:HD11	3:L:213:ILE:HG21	1.67	0.77
1:M:598:LEU:HD23	1:M:601:ARG:HD2	1.66	0.77
1:G:598:LEU:HD23	1:G:601:ARG:HD2	1.65	0.76
2:Q:410:ARG:HA	2:Q:413:LEU:HB3	1.66	0.76
1:J:353:ASP:OD1	1:J:379:LYS:NZ	2.18	0.76
1:P:598:LEU:HD23	1:P:601:ARG:HD2	1.66	0.76
1:A:598:LEU:HD23	1:A:601:ARG:HD2	1.65	0.76
1:M:353:ASP:OD1	1:M:379:LYS:NZ	2.19	0.76
2:E:410:ARG:HA	2:E:413:LEU:HB3	1.66	0.75
3:F:242:ILE:HG22	3:F:245:VAL:HG22	1.68	0.75
3:O:252:GLY:O	3:O:256:GLU:HB2	1.87	0.75
3:I:242:ILE:HG22	3:I:245:VAL:HG22	1.68	0.75
2:N:410:ARG:HA	2:N:413:LEU:HB3	1.66	0.75
1:G:436:ILE:HD12	3:I:143:THR:HG23	1.67	0.75
3:R:242:ILE:HG22	3:R:245:VAL:HG22	1.68	0.75
3:R:347:ASP:O	3:R:351:GLU:HB2	1.87	0.75
3:F:347:ASP:O	3:F:351:GLU:HB2	1.87	0.75
1:A:436:ILE:HD12	3:C:143:THR:HG23	1.67	0.75
1:M:436:ILE:HD12	3:O:143:THR:HG23	1.67	0.75
3:O:347:ASP:O	3:O:351:GLU:HB2	1.87	0.75
3:R:252:GLY:O	3:R:256:GLU:HB2	1.87	0.74
3:C:252:GLY:O	3:C:256:GLU:HB2	1.86	0.74
3:I:252:GLY:O	3:I:256:GLU:HB2	1.86	0.74
3:I:347:ASP:O	3:I:351:GLU:HB2	1.87	0.74
1:J:436:ILE:HD12	3:L:143:THR:HG23	1.68	0.74
1:P:428:GLU:HB2	1:P:435:ARG:HH12	1.53	0.74
3:C:242:ILE:HG22	3:C:245:VAL:HG22	1.68	0.74
3:I:6:ILE:HD11	3:I:213:ILE:HG21	1.70	0.74
3:L:252:GLY:O	3:L:256:GLU:HB2	1.86	0.74
1:D:353:ASP:OD1	1:D:379:LYS:NZ	2.20	0.74
1:J:405:TYR:CE1	1:J:414:ILE:HG23	2.23	0.74
3:O:242:ILE:HG22	3:O:245:VAL:HG22	1.68	0.74
3:C:347:ASP:O	3:C:351:GLU:HB2	1.87	0.74
3:F:414:PHE:HA	3:F:417:ILE:HG22	1.69	0.74
3:I:414:PHE:HA	3:I:417:ILE:HG22	1.69	0.74
1:M:428:GLU:HB2	1:M:435:ARG:HH12	1.52	0.74
2:N:208:PRO:HG2	2:N:211:TYR:HD2	1.53	0.74
1:A:323:ASN:HA	1:A:350:THR:HA	1.71	0.73
3:F:6:ILE:HD11	3:F:213:ILE:HG21	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:252:GLY:O	3:F:256:GLU:HB2	1.87	0.73
3:L:347:ASP:O	3:L:351:GLU:HB2	1.87	0.73
1:G:353:ASP:OD1	1:G:379:LYS:NZ	2.21	0.73
3:L:242:ILE:HG22	3:L:245:VAL:HG22	1.68	0.73
2:Q:208:PRO:HG2	2:Q:211:TYR:HD2	1.54	0.73
2:E:208:PRO:HG2	2:E:211:TYR:HD2	1.53	0.73
3:O:6:ILE:HD11	3:O:213:ILE:HG21	1.69	0.73
3:R:6:ILE:HD11	3:R:213:ILE:HG21	1.69	0.73
1:D:662:LEU:HB3	1:D:665:ASN:HD21	1.54	0.73
1:J:428:GLU:HB2	1:J:435:ARG:HH12	1.53	0.73
1:P:353:ASP:OD1	1:P:379:LYS:NZ	2.21	0.73
1:D:436:ILE:HD12	3:F:143:THR:HG23	1.69	0.73
1:P:405:TYR:CE1	1:P:414:ILE:HG23	2.23	0.73
1:A:271:ILE:O	1:A:289:SER:HB3	1.89	0.73
3:C:6:ILE:HD11	3:C:213:ILE:HG21	1.70	0.73
1:D:428:GLU:HB2	1:D:435:ARG:HH12	1.53	0.73
2:K:208:PRO:HG2	2:K:211:TYR:HD2	1.53	0.73
1:A:375:PHE:CE1	1:A:380:MET:HG3	2.24	0.73
1:G:428:GLU:HB2	1:G:435:ARG:HH12	1.53	0.73
3:O:414:PHE:HA	3:O:417:ILE:HG22	1.69	0.73
1:D:405:TYR:CE1	1:D:414:ILE:HG23	2.23	0.72
3:L:414:PHE:HA	3:L:417:ILE:HG22	1.69	0.72
3:R:414:PHE:HA	3:R:417:ILE:HG22	1.69	0.72
1:M:775:TRP:H	2:N:109:GLN:HE22	1.36	0.72
1:P:271:ILE:O	1:P:289:SER:HB3	1.88	0.72
1:M:375:PHE:CE1	1:M:380:MET:HG3	2.25	0.72
1:A:353:ASP:OD1	1:A:379:LYS:NZ	2.21	0.72
1:M:323:ASN:HA	1:M:350:THR:HA	1.71	0.72
1:A:405:TYR:CE1	1:A:414:ILE:HG23	2.24	0.72
2:H:208:PRO:HG2	2:H:211:TYR:HD2	1.53	0.72
1:M:405:TYR:CE1	1:M:414:ILE:HG23	2.24	0.72
1:A:428:GLU:HB2	1:A:435:ARG:HH12	1.53	0.72
1:G:775:TRP:H	2:H:109:GLN:HE22	1.36	0.72
1:J:375:PHE:CE1	1:J:380:MET:HG3	2.24	0.72
1:M:625:ASP:O	1:M:629:ARG:HB3	1.90	0.72
3:O:75:GLN:HA	3:O:78:ARG:HE	1.55	0.72
2:Q:378:LEU:HD21	3:R:235:ILE:HD13	1.72	0.72
1:M:271:ILE:O	1:M:289:SER:HB3	1.89	0.72
1:P:662:LEU:HB3	1:P:665:ASN:HD21	1.54	0.72
3:C:75:GLN:HA	3:C:78:ARG:HE	1.55	0.72
1:P:384:ASP:HB3	1:P:389:TRP:HB3	1.72	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:323:ASN:HA	1:J:350:THR:HA	1.71	0.72
2:B:208:PRO:HG2	2:B:211:TYR:HD2	1.53	0.71
1:D:271:ILE:O	1:D:289:SER:HB3	1.90	0.71
1:G:662:LEU:HB3	1:G:665:ASN:HD21	1.55	0.71
1:J:271:ILE:O	1:J:289:SER:HB3	1.89	0.71
1:D:323:ASN:HA	1:D:350:THR:HA	1.71	0.71
3:R:75:GLN:HA	3:R:78:ARG:HE	1.55	0.71
1:M:302:VAL:HG21	1:M:362:ARG:HD2	1.72	0.71
1:P:375:PHE:CE1	1:P:380:MET:HG3	2.24	0.71
1:P:625:ASP:O	1:P:629:ARG:HB3	1.90	0.71
3:I:75:GLN:HA	3:I:78:ARG:HE	1.55	0.71
3:C:414:PHE:HA	3:C:417:ILE:HG22	1.69	0.71
1:D:364:GLU:O	1:D:373:LEU:HB2	1.91	0.71
1:D:375:PHE:CE1	1:D:380:MET:HG3	2.24	0.71
1:D:384:ASP:HB3	1:D:389:TRP:HB3	1.72	0.71
1:G:384:ASP:HB3	1:G:389:TRP:HB3	1.71	0.71
1:J:625:ASP:O	1:J:629:ARG:HB3	1.90	0.71
3:F:75:GLN:HA	3:F:78:ARG:HE	1.55	0.71
1:G:405:TYR:CE1	1:G:414:ILE:HG23	2.23	0.71
3:L:75:GLN:HA	3:L:78:ARG:HE	1.55	0.71
1:P:323:ASN:HA	1:P:350:THR:HA	1.71	0.71
1:G:625:ASP:O	1:G:629:ARG:HB3	1.90	0.71
1:J:384:ASP:HB3	1:J:389:TRP:HB3	1.71	0.71
1:G:323:ASN:HA	1:G:350:THR:HA	1.71	0.71
1:G:53:ASP:OD2	1:G:54:ALA:N	2.23	0.71
1:P:53:ASP:OD2	1:P:54:ALA:N	2.24	0.71
1:D:625:ASP:O	1:D:629:ARG:HB3	1.90	0.71
1:J:364:GLU:O	1:J:373:LEU:HB2	1.91	0.71
2:K:411:ARG:O	2:K:415:LYS:HB2	1.91	0.71
1:M:662:LEU:HB3	1:M:665:ASN:HD21	1.54	0.71
2:E:411:ARG:O	2:E:415:LYS:HB2	1.91	0.70
1:G:375:PHE:CE1	1:G:380:MET:HG3	2.24	0.70
3:I:161:ASN:HA	3:I:164:LYS:HD2	1.73	0.70
1:A:302:VAL:HG21	1:A:362:ARG:HD2	1.71	0.70
1:A:384:ASP:HB3	1:A:389:TRP:HB3	1.72	0.70
1:D:446:ASP:OD2	1:D:448:THR:HG22	1.92	0.70
2:H:411:ARG:O	2:H:415:LYS:HB2	1.91	0.70
1:J:53:ASP:OD2	1:J:54:ALA:N	2.23	0.70
1:M:384:ASP:HB3	1:M:389:TRP:HB3	1.72	0.70
1:P:659:LEU:HD13	1:P:659:LEU:H	1.56	0.70
1:A:625:ASP:O	1:A:629:ARG:HB3	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:662:LEU:HB3	1:A:665:ASN:HD21	1.55	0.70
1:G:302:VAL:HG21	1:G:362:ARG:HD2	1.71	0.70
1:P:302:VAL:HG11	1:P:362:ARG:HH11	1.56	0.70
1:A:302:VAL:HG11	1:A:362:ARG:HH11	1.56	0.70
1:A:53:ASP:OD2	1:A:54:ALA:N	2.24	0.70
2:B:411:ARG:O	2:B:415:LYS:HB2	1.92	0.70
1:D:659:LEU:HD13	1:D:659:LEU:H	1.56	0.70
1:P:532:GLU:HA	1:P:554:ASN:HD22	1.56	0.70
1:J:717:LYS:NZ	4:J:1003:SO4:O1	2.23	0.70
1:M:302:VAL:HG11	1:M:362:ARG:HH11	1.56	0.70
1:G:659:LEU:HD13	1:G:659:LEU:H	1.56	0.70
1:J:446:ASP:OD2	1:J:448:THR:HG22	1.92	0.70
1:P:302:VAL:HG21	1:P:362:ARG:HD2	1.72	0.70
1:G:532:GLU:HA	1:G:554:ASN:HD22	1.57	0.70
2:H:139:LYS:HG2	2:H:237:ILE:HG12	1.74	0.70
1:D:302:VAL:HG21	1:D:362:ARG:HD2	1.72	0.70
3:L:161:ASN:HA	3:L:164:LYS:HD2	1.74	0.70
1:M:53:ASP:OD2	1:M:54:ALA:N	2.23	0.70
2:N:411:ARG:O	2:N:415:LYS:HB2	1.92	0.70
2:Q:411:ARG:O	2:Q:415:LYS:HB2	1.91	0.70
1:D:532:GLU:HA	1:D:554:ASN:HD22	1.57	0.70
2:E:378:LEU:HD21	3:F:235:ILE:HD13	1.73	0.70
1:J:532:GLU:HA	1:J:554:ASN:HD22	1.57	0.70
1:J:662:LEU:HB3	1:J:665:ASN:HD21	1.55	0.70
1:P:358:SER:HB3	1:P:377:ARG:HD3	1.74	0.70
3:R:171:ARG:O	3:R:174:GLU:N	2.25	0.70
1:G:271:ILE:O	1:G:289:SER:HB3	1.90	0.69
2:N:139:LYS:HG2	2:N:237:ILE:HG12	1.74	0.69
1:P:364:GLU:O	1:P:373:LEU:HB2	1.92	0.69
2:B:139:LYS:HG2	2:B:237:ILE:HG12	1.74	0.69
1:D:302:VAL:HG11	1:D:362:ARG:HH11	1.56	0.69
1:G:358:SER:HB3	1:G:377:ARG:HD3	1.74	0.69
1:A:364:GLU:O	1:A:373:LEU:HB2	1.93	0.69
1:A:532:GLU:HA	1:A:554:ASN:HD22	1.57	0.69
1:A:662:LEU:HB3	1:A:665:ASN:ND2	2.07	0.69
1:M:532:GLU:HA	1:M:554:ASN:HD22	1.56	0.69
3:C:161:ASN:HA	3:C:164:LYS:HD2	1.74	0.69
2:E:139:LYS:HG2	2:E:237:ILE:HG12	1.74	0.69
1:J:302:VAL:HG21	1:J:362:ARG:HD2	1.73	0.69
1:M:659:LEU:HD13	1:M:659:LEU:H	1.57	0.69
1:A:775:TRP:H	2:B:109:GLN:HE22	1.38	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:288:GLU:O	2:B:290:THR:OG1	2.11	0.69
1:D:358:SER:HB3	1:D:377:ARG:HD3	1.75	0.69
1:D:53:ASP:OD2	1:D:54:ALA:N	2.24	0.69
2:N:378:LEU:HD21	3:O:235:ILE:HD13	1.74	0.69
1:D:717:LYS:NZ	4:D:1004:SO4:O1	2.24	0.69
1:G:446:ASP:OD2	1:G:448:THR:HG22	1.93	0.69
1:J:358:SER:HB3	1:J:377:ARG:HD3	1.75	0.69
1:M:364:GLU:O	1:M:373:LEU:HB2	1.92	0.69
3:F:373:LEU:HD12	3:F:411:VAL:HG21	1.75	0.69
1:A:659:LEU:HD13	1:A:659:LEU:H	1.57	0.69
1:G:364:GLU:O	1:G:373:LEU:HB2	1.93	0.69
1:J:659:LEU:HD13	1:J:659:LEU:H	1.57	0.69
1:M:662:LEU:HB3	1:M:665:ASN:ND2	2.07	0.69
1:P:662:LEU:HB3	1:P:665:ASN:ND2	2.07	0.69
1:J:302:VAL:HG11	1:J:362:ARG:HH11	1.56	0.69
3:I:313:LEU:HG	3:I:367:ILE:HG21	1.75	0.69
2:N:288:GLU:O	2:N:290:THR:OG1	2.10	0.69
3:C:373:LEU:HD12	3:C:411:VAL:HG21	1.75	0.68
1:D:622:TYR:CZ	1:D:668:SER:HB3	2.28	0.68
1:G:302:VAL:HG11	1:G:362:ARG:HH11	1.57	0.68
2:K:139:LYS:HG2	2:K:237:ILE:HG12	1.74	0.68
3:L:373:LEU:HD12	3:L:411:VAL:HG21	1.75	0.68
3:R:313:LEU:HG	3:R:367:ILE:HG21	1.74	0.68
1:A:405:TYR:HB2	1:A:416:LEU:HD12	1.76	0.68
1:J:775:TRP:H	2:K:109:GLN:HE22	1.38	0.68
2:K:113:LYS:HG3	2:K:134:LYS:HZ1	1.59	0.68
3:C:171:ARG:O	3:C:174:GLU:N	2.25	0.68
3:F:161:ASN:HA	3:F:164:LYS:HD2	1.75	0.68
2:H:288:GLU:O	2:H:290:THR:OG1	2.11	0.68
3:R:161:ASN:HA	3:R:164:LYS:HD2	1.75	0.68
1:A:358:SER:HB3	1:A:377:ARG:HD3	1.75	0.68
1:P:775:TRP:H	2:Q:109:GLN:HE22	1.39	0.68
2:Q:139:LYS:HG2	2:Q:237:ILE:HG12	1.75	0.68
1:A:584:ARG:O	1:A:588:SER:HB2	1.92	0.68
3:C:427:PRO:HG2	3:C:429:ARG:HG2	1.75	0.68
3:I:1:MET:N	3:I:218:ASP:OD2	2.23	0.68
2:H:378:LEU:HD21	3:I:235:ILE:HD13	1.74	0.68
3:O:161:ASN:HA	3:O:164:LYS:HD2	1.75	0.68
1:D:408:ILE:HG22	1:D:415:LEU:HB2	1.75	0.68
3:F:171:ARG:O	3:F:174:GLU:N	2.26	0.68
1:J:408:ILE:HG22	1:J:415:LEU:HB2	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:446:ASP:OD2	1:A:448:THR:HG22	1.93	0.68
1:M:446:ASP:OD2	1:M:448:THR:HG22	1.93	0.68
3:O:171:ARG:O	3:O:174:GLU:N	2.27	0.68
1:P:584:ARG:O	1:P:588:SER:HB2	1.94	0.68
1:A:345:ASP:N	1:A:345:ASP:OD1	2.25	0.68
1:D:662:LEU:HB3	1:D:665:ASN:ND2	2.07	0.68
3:F:313:LEU:HG	3:F:367:ILE:HG21	1.75	0.68
1:M:622:TYR:CZ	1:M:668:SER:HB3	2.29	0.68
1:M:675:PHE:HE2	1:M:741:ILE:HG21	1.58	0.68
1:P:446:ASP:OD2	1:P:448:THR:HG22	1.93	0.68
1:G:675:PHE:HE2	1:G:741:ILE:HG21	1.58	0.68
1:J:662:LEU:HB3	1:J:665:ASN:ND2	2.07	0.68
2:K:288:GLU:O	2:K:290:THR:OG1	2.11	0.68
1:M:584:ARG:O	1:M:588:SER:HB2	1.94	0.68
1:J:412:ASN:OD1	1:J:412:ASN:N	2.27	0.68
2:K:366:TYR:HA	2:K:369:TRP:NE1	2.09	0.68
3:L:427:PRO:HG2	3:L:429:ARG:HG2	1.75	0.68
1:P:177:THR:HG22	1:P:301:GLN:HE22	1.59	0.68
2:Q:288:GLU:O	2:Q:290:THR:OG1	2.11	0.68
1:D:412:ASN:N	1:D:412:ASN:OD1	2.27	0.67
1:G:177:THR:HG22	1:G:301:GLN:HE22	1.60	0.67
1:J:584:ARG:O	1:J:588:SER:HB2	1.93	0.67
1:M:405:TYR:HB2	1:M:416:LEU:HD12	1.76	0.67
2:N:283:ASN:OD1	2:N:284:LEU:N	2.27	0.67
3:O:313:LEU:HG	3:O:367:ILE:HG21	1.75	0.67
3:O:427:PRO:HG2	3:O:429:ARG:HG2	1.75	0.67
1:P:345:ASP:OD1	1:P:345:ASP:N	2.26	0.67
1:P:408:ILE:HG22	1:P:415:LEU:HB2	1.76	0.67
3:C:313:LEU:HG	3:C:367:ILE:HG21	1.75	0.67
1:D:322:GLY:O	1:D:351:ILE:N	2.23	0.67
1:D:345:ASP:OD1	1:D:345:ASP:N	2.26	0.67
3:F:427:PRO:HG2	3:F:429:ARG:HG2	1.75	0.67
1:G:330:PRO:HG3	1:G:342:GLN:HG3	1.76	0.67
1:G:408:ILE:HG22	1:G:415:LEU:HB2	1.75	0.67
3:L:313:LEU:HG	3:L:367:ILE:HG21	1.74	0.67
1:M:408:ILE:HG22	1:M:415:LEU:HB2	1.76	0.67
1:A:330:PRO:HG3	1:A:342:GLN:HG3	1.75	0.67
1:A:412:ASN:N	1:A:412:ASN:OD1	2.26	0.67
2:B:366:TYR:HA	2:B:369:TRP:NE1	2.10	0.67
1:D:177:THR:HG22	1:D:301:GLN:HE22	1.60	0.67
1:G:775:TRP:H	2:H:109:GLN:NE2	1.93	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:330:PRO:HG3	1:J:342:GLN:HG3	1.76	0.67
1:M:412:ASN:OD1	1:M:412:ASN:N	2.27	0.67
1:G:412:ASN:N	1:G:412:ASN:OD1	2.26	0.67
1:G:698:LYS:HE2	2:H:124:ARG:HH21	1.58	0.67
1:M:177:THR:HG22	1:M:301:GLN:HE22	1.59	0.67
1:D:775:TRP:H	2:E:109:GLN:HE22	1.40	0.67
1:P:675:PHE:HE2	1:P:741:ILE:HG21	1.58	0.67
1:A:675:PHE:HE2	1:A:741:ILE:HG21	1.59	0.67
1:D:584:ARG:O	1:D:588:SER:HB2	1.94	0.67
1:J:675:PHE:HE2	1:J:741:ILE:HG21	1.59	0.67
2:N:366:TYR:HA	2:N:369:TRP:NE1	2.09	0.67
2:H:290:THR:HB	2:H:292:GLU:H	1.60	0.67
1:M:358:SER:HB3	1:M:377:ARG:HD3	1.76	0.67
1:P:405:TYR:HB2	1:P:416:LEU:HD12	1.75	0.67
3:R:373:LEU:HD12	3:R:411:VAL:HG21	1.76	0.67
1:A:177:THR:HG22	1:A:301:GLN:HE22	1.59	0.67
1:G:662:LEU:HB3	1:G:665:ASN:ND2	2.08	0.67
2:K:290:THR:HB	2:K:292:GLU:H	1.60	0.67
2:Q:366:TYR:HA	2:Q:369:TRP:NE1	2.10	0.67
2:B:378:LEU:HD21	3:C:235:ILE:HD13	1.75	0.67
2:E:162:ILE:HG21	2:E:226:LEU:HD11	1.76	0.67
1:G:322:GLY:O	1:G:351:ILE:N	2.24	0.67
1:G:584:ARG:O	1:G:588:SER:HB2	1.94	0.67
1:J:383:ILE:HG12	1:J:390:GLN:HG2	1.77	0.67
1:M:345:ASP:N	1:M:345:ASP:OD1	2.27	0.67
1:P:322:GLY:O	1:P:351:ILE:N	2.24	0.67
2:Q:162:ILE:HG21	2:Q:226:LEU:HD11	1.77	0.67
2:Q:290:THR:HB	2:Q:292:GLU:H	1.60	0.67
3:R:1:MET:N	3:R:218:ASP:OD2	2.28	0.67
1:A:232:ASN:ND2	1:A:282:CYS:O	2.23	0.67
2:B:290:THR:HB	2:B:292:GLU:H	1.60	0.67
2:E:290:THR:HB	2:E:292:GLU:H	1.60	0.67
1:G:405:TYR:HB2	1:G:416:LEU:HD12	1.76	0.67
1:J:345:ASP:N	1:J:345:ASP:OD1	2.26	0.67
1:A:383:ILE:HG12	1:A:390:GLN:HG2	1.77	0.66
1:D:675:PHE:HE2	1:D:741:ILE:HG21	1.59	0.66
2:E:288:GLU:O	2:E:290:THR:OG1	2.11	0.66
2:H:283:ASN:OD1	2:H:284:LEU:N	2.27	0.66
3:I:373:LEU:HD12	3:I:411:VAL:HG21	1.76	0.66
1:M:330:PRO:HG3	1:M:342:GLN:HG3	1.76	0.66
1:P:330:PRO:HG3	1:P:342:GLN:HG3	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:405:TYR:HB2	1:D:416:LEU:HD12	1.77	0.66
2:E:113:LYS:HG3	2:E:134:LYS:HZ1	1.61	0.66
2:E:183:LYS:O	2:E:187:THR:OG1	2.13	0.66
3:I:171:ARG:O	3:I:174:GLU:N	2.27	0.66
3:L:171:ARG:O	3:L:174:GLU:N	2.26	0.66
3:L:1:MET:N	3:L:218:ASP:OD2	2.26	0.66
1:M:697:GLU:N	1:M:697:GLU:OE1	2.28	0.66
1:P:700:LEU:HD12	1:P:703:PHE:HD2	1.61	0.66
1:A:473:HIS:CD2	1:A:475:ARG:HD2	2.31	0.66
1:D:232:ASN:ND2	1:D:282:CYS:O	2.23	0.66
2:E:366:TYR:HA	2:E:369:TRP:NE1	2.10	0.66
2:H:104:PHE:CZ	2:H:156:LEU:HB2	2.31	0.66
2:K:183:LYS:O	2:K:187:THR:OG1	2.13	0.66
1:M:775:TRP:H	2:N:109:GLN:NE2	1.93	0.66
1:P:622:TYR:CZ	1:P:668:SER:HB3	2.31	0.66
1:J:177:THR:HG22	1:J:301:GLN:HE22	1.60	0.66
3:O:373:LEU:HD12	3:O:411:VAL:HG21	1.76	0.66
1:A:408:ILE:HG22	1:A:415:LEU:HB2	1.76	0.66
1:J:232:ASN:ND2	1:J:282:CYS:O	2.23	0.66
1:J:405:TYR:HB2	1:J:416:LEU:HD12	1.76	0.66
1:M:717:LYS:NZ	4:M:1004:SO4:O1	2.29	0.66
3:R:427:PRO:HG2	3:R:429:ARG:HG2	1.76	0.66
1:G:49:THR:HB	3:I:318:ILE:HG21	1.76	0.66
2:H:113:LYS:HG3	2:H:134:LYS:HZ1	1.60	0.66
2:H:183:LYS:O	2:H:187:THR:OG1	2.12	0.66
2:N:162:ILE:HG21	2:N:226:LEU:HD11	1.77	0.66
2:N:290:THR:HB	2:N:292:GLU:H	1.61	0.66
2:H:503:SER:O	2:H:507:ASN:ND2	2.29	0.66
1:M:383:ILE:HG12	1:M:390:GLN:HG2	1.78	0.66
2:B:208:PRO:HG2	2:B:211:TYR:CD2	2.31	0.66
3:I:427:PRO:HG2	3:I:429:ARG:HG2	1.76	0.66
2:K:104:PHE:CZ	2:K:156:LEU:HB2	2.31	0.66
2:K:378:LEU:HD21	3:L:235:ILE:HD13	1.76	0.66
2:B:183:LYS:O	2:B:187:THR:OG1	2.13	0.66
2:B:283:ASN:OD1	2:B:284:LEU:N	2.27	0.66
1:D:330:PRO:HG3	1:D:342:GLN:HG3	1.76	0.66
1:D:700:LEU:HD12	1:D:703:PHE:HD2	1.61	0.66
1:M:232:ASN:ND2	1:M:282:CYS:O	2.23	0.66
1:P:383:ILE:HG12	1:P:390:GLN:HG2	1.78	0.66
1:D:383:ILE:HG12	1:D:390:GLN:HG2	1.78	0.66
2:K:436:LEU:HD12	2:K:436:LEU:H	1.60	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:698:LYS:HE2	2:N:124:ARG:HH21	1.60	0.66
2:Q:104:PHE:CZ	2:Q:156:LEU:HB2	2.30	0.66
1:G:232:ASN:ND2	1:G:282:CYS:O	2.23	0.65
2:H:366:TYR:HA	2:H:369:TRP:NE1	2.10	0.65
1:P:719:LEU:HD13	1:P:733:THR:HG21	1.78	0.65
1:A:622:TYR:CZ	1:A:668:SER:HB3	2.31	0.65
1:D:67:ASP:OD1	1:D:545:SER:OG	2.13	0.65
1:M:473:HIS:CD2	1:M:475:ARG:HD2	2.31	0.65
1:P:412:ASN:N	1:P:412:ASN:OD1	2.27	0.65
3:C:1:MET:N	3:C:218:ASP:OD2	2.27	0.65
2:E:104:PHE:CZ	2:E:156:LEU:HB2	2.31	0.65
1:P:698:LYS:HE2	2:Q:124:ARG:HH21	1.62	0.65
2:Q:113:LYS:HG3	2:Q:134:LYS:HZ1	1.61	0.65
1:G:622:TYR:CZ	1:G:668:SER:HB3	2.32	0.65
2:K:208:PRO:HG2	2:K:211:TYR:CD2	2.31	0.65
1:P:717:LYS:NZ	4:P:1005:SO4:O1	2.28	0.65
1:A:697:GLU:OE1	1:A:697:GLU:N	2.29	0.65
2:E:503:SER:O	2:E:507:ASN:ND2	2.29	0.65
1:J:473:HIS:CD2	1:J:475:ARG:HD2	2.31	0.65
1:M:700:LEU:HD12	1:M:703:PHE:HD2	1.61	0.65
2:Q:183:LYS:O	2:Q:187:THR:OG1	2.13	0.65
2:B:113:LYS:HG3	2:B:134:LYS:HZ1	1.62	0.65
1:J:622:TYR:CZ	1:J:668:SER:HB3	2.32	0.65
2:N:183:LYS:O	2:N:187:THR:OG1	2.14	0.65
2:N:208:PRO:HG2	2:N:211:TYR:CD2	2.31	0.65
2:B:104:PHE:CZ	2:B:156:LEU:HB2	2.31	0.65
1:A:698:LYS:HE2	2:B:124:ARG:HH21	1.61	0.65
1:G:383:ILE:HG12	1:G:390:GLN:HG2	1.79	0.65
2:E:436:LEU:HD12	2:E:436:LEU:H	1.61	0.65
1:G:700:LEU:HD12	1:G:703:PHE:HD2	1.62	0.65
1:P:49:THR:HB	3:R:318:ILE:HG21	1.77	0.65
1:A:484:ARG:O	1:A:486:ALA:N	2.30	0.65
1:A:625:ASP:O	1:A:629:ARG:CB	2.45	0.65
2:E:283:ASN:OD1	2:E:284:LEU:N	2.27	0.65
1:G:345:ASP:N	1:G:345:ASP:OD1	2.27	0.65
2:H:208:PRO:HG2	2:H:211:TYR:CD2	2.31	0.65
2:K:503:SER:O	2:K:507:ASN:ND2	2.30	0.65
2:N:503:SER:O	2:N:507:ASN:ND2	2.30	0.65
2:E:208:PRO:HG2	2:E:211:TYR:CD2	2.31	0.65
1:G:717:LYS:NZ	4:G:903:SO4:O1	2.29	0.65
1:J:49:THR:HB	3:L:318:ILE:HG21	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:283:ASN:OD1	2:Q:284:LEU:N	2.27	0.65
1:D:473:HIS:CD2	1:D:475:ARG:HD2	2.31	0.64
1:D:697:GLU:N	1:D:697:GLU:OE1	2.29	0.64
3:F:369:ALA:HB1	3:F:411:VAL:HG23	1.79	0.64
1:J:479:HIS:NE2	1:J:491:SER:OG	2.23	0.64
2:N:113:LYS:HG3	2:N:134:LYS:HZ1	1.62	0.64
2:Q:245:SER:HB3	2:Q:284:LEU:HB2	1.79	0.64
1:D:698:LYS:HE2	2:E:124:ARG:HH21	1.63	0.64
2:H:245:SER:HB3	2:H:284:LEU:HB2	1.79	0.64
2:H:361:PRO:O	2:H:364:SER:N	2.30	0.64
1:J:625:ASP:O	1:J:629:ARG:CB	2.46	0.64
1:M:719:LEU:HD13	1:M:733:THR:HG21	1.79	0.64
2:Q:208:PRO:HG2	2:Q:211:TYR:CD2	2.31	0.64
1:D:269:PHE:HB2	1:D:300:LEU:HD11	1.80	0.64
1:D:49:THR:HB	3:F:318:ILE:HG21	1.78	0.64
1:J:700:LEU:HD12	1:J:703:PHE:HD2	1.61	0.64
1:J:775:TRP:H	2:K:109:GLN:NE2	1.95	0.64
2:B:503:SER:O	2:B:507:ASN:ND2	2.30	0.64
1:J:698:LYS:HE2	2:K:124:ARG:HH21	1.61	0.64
2:K:162:ILE:HG21	2:K:226:LEU:HD11	1.78	0.64
2:N:104:PHE:CZ	2:N:156:LEU:HB2	2.31	0.64
1:A:656:HIS:CD2	1:A:656:HIS:H	2.14	0.64
1:D:719:LEU:HD13	1:D:733:THR:HG21	1.80	0.64
2:H:162:ILE:HG21	2:H:226:LEU:HD11	1.77	0.64
1:J:719:LEU:HD13	1:J:733:THR:HG21	1.80	0.64
1:M:422:ILE:O	1:M:439:LYS:HB2	1.97	0.64
1:A:717:LYS:NZ	4:A:1005:SO4:O1	2.28	0.64
1:A:49:THR:HB	3:C:318:ILE:HG21	1.79	0.64
1:G:625:ASP:O	1:G:629:ARG:CB	2.45	0.64
1:D:625:ASP:O	1:D:629:ARG:CB	2.45	0.64
1:J:484:ARG:O	1:J:486:ALA:N	2.31	0.64
1:P:775:TRP:H	2:Q:109:GLN:NE2	1.95	0.64
1:A:775:TRP:H	2:B:109:GLN:NE2	1.95	0.64
2:E:361:PRO:O	2:E:364:SER:N	2.31	0.64
1:G:473:HIS:CD2	1:G:475:ARG:HD2	2.32	0.64
1:M:405:TYR:OH	1:M:414:ILE:HG12	1.98	0.64
2:B:361:PRO:O	2:B:364:SER:N	2.30	0.64
1:D:479:HIS:NE2	1:D:491:SER:OG	2.24	0.64
1:J:269:PHE:HB2	1:J:300:LEU:HD11	1.80	0.64
1:J:422:ILE:HG12	1:J:442:LEU:HD12	1.80	0.64
1:P:269:PHE:HB2	1:P:300:LEU:HD11	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:719:LEU:HD13	1:G:733:THR:HG21	1.80	0.64
1:M:49:THR:HB	3:O:318:ILE:HG21	1.80	0.64
1:P:473:HIS:CD2	1:P:475:ARG:HD2	2.33	0.64
1:A:269:PHE:HB2	1:A:300:LEU:HD11	1.79	0.63
1:A:405:TYR:OH	1:A:414:ILE:HG12	1.98	0.63
1:D:321:LYS:HA	1:D:361:LYS:HD3	1.79	0.63
3:F:1:MET:N	3:F:218:ASP:OD2	2.30	0.63
1:J:656:HIS:CD2	1:J:656:HIS:H	2.15	0.63
1:M:625:ASP:O	1:M:629:ARG:CB	2.46	0.63
2:N:245:SER:HB3	2:N:284:LEU:HB2	1.80	0.63
1:P:405:TYR:OH	1:P:414:ILE:HG12	1.98	0.63
1:P:422:ILE:O	1:P:439:LYS:HB2	1.98	0.63
3:R:369:ALA:HB1	3:R:411:VAL:HG23	1.80	0.63
1:A:719:LEU:HD13	1:A:733:THR:HG21	1.80	0.63
1:M:656:HIS:CD2	1:M:656:HIS:H	2.15	0.63
2:N:361:PRO:O	2:N:364:SER:N	2.31	0.63
1:P:625:ASP:O	1:P:629:ARG:CB	2.45	0.63
2:Q:361:PRO:O	2:Q:364:SER:N	2.31	0.63
1:D:405:TYR:OH	1:D:414:ILE:HG12	1.98	0.63
1:G:405:TYR:OH	1:G:414:ILE:HG12	1.98	0.63
1:G:422:ILE:O	1:G:439:LYS:HB2	1.98	0.63
1:J:321:LYS:HA	1:J:361:LYS:HD3	1.80	0.63
1:M:503:GLY:O	1:M:504:THR:OG1	2.16	0.63
1:A:422:ILE:O	1:A:439:LYS:HB2	1.98	0.63
1:G:484:ARG:O	1:G:486:ALA:N	2.31	0.63
1:J:405:TYR:OH	1:J:414:ILE:HG12	1.97	0.63
1:A:67:ASP:OD1	1:A:545:SER:OG	2.16	0.63
2:B:436:LEU:H	2:B:436:LEU:HD12	1.62	0.63
2:H:436:LEU:HD12	2:H:436:LEU:H	1.64	0.63
2:K:361:PRO:O	2:K:364:SER:N	2.31	0.63
1:A:271:ILE:O	1:A:289:SER:CB	2.47	0.63
1:A:321:LYS:HA	1:A:361:LYS:HD3	1.80	0.63
1:A:422:ILE:HG12	1:A:442:LEU:HD12	1.80	0.63
1:D:422:ILE:HG12	1:D:442:LEU:HD12	1.80	0.63
1:D:484:ARG:O	1:D:486:ALA:N	2.31	0.63
2:E:245:SER:HB3	2:E:284:LEU:HB2	1.79	0.63
1:G:573:GLU:HB2	2:H:499:LYS:HZ3	1.64	0.63
1:M:422:ILE:HG12	1:M:442:LEU:HD12	1.80	0.63
3:O:369:ALA:HB1	3:O:411:VAL:HG23	1.79	0.63
1:P:484:ARG:O	1:P:486:ALA:N	2.31	0.63
1:D:775:TRP:H	2:E:109:GLN:NE2	1.95	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:369:ALA:HB1	3:L:411:VAL:HG23	1.80	0.63
1:M:484:ARG:O	1:M:486:ALA:N	2.31	0.63
2:N:436:LEU:H	2:N:436:LEU:HD12	1.62	0.63
3:O:361:ASP:HB3	3:O:364:VAL:HG13	1.80	0.63
1:P:656:HIS:CD2	1:P:656:HIS:H	2.15	0.63
1:J:375:PHE:HD1	1:J:402:ILE:HD13	1.63	0.63
2:B:162:ILE:HG21	2:B:226:LEU:HD11	1.79	0.62
3:C:303:THR:HG22	3:C:304:HIS:H	1.64	0.62
2:K:245:SER:HB3	2:K:284:LEU:HB2	1.80	0.62
1:M:269:PHE:HB2	1:M:300:LEU:HD11	1.80	0.62
1:P:232:ASN:ND2	1:P:282:CYS:O	2.23	0.62
3:R:412:ARG:NH2	3:R:439:GLU:OE2	2.32	0.62
1:A:700:LEU:HD12	1:A:703:PHE:HD2	1.62	0.62
3:I:369:ALA:HB1	3:I:411:VAL:HG23	1.81	0.62
2:Q:436:LEU:H	2:Q:436:LEU:HD12	1.62	0.62
1:A:503:GLY:O	1:A:504:THR:OG1	2.16	0.62
1:A:662:LEU:O	1:A:665:ASN:ND2	2.32	0.62
3:F:412:ARG:NH2	3:F:439:GLU:OE2	2.32	0.62
1:G:321:LYS:HA	1:G:361:LYS:HD3	1.80	0.62
1:P:271:ILE:O	1:P:289:SER:CB	2.47	0.62
1:P:422:ILE:HG12	1:P:442:LEU:HD12	1.80	0.62
2:B:245:SER:HB3	2:B:284:LEU:HB2	1.79	0.62
1:D:365:TRP:HB2	1:D:371:LYS:O	2.00	0.62
1:G:422:ILE:HG12	1:G:442:LEU:HD12	1.80	0.62
1:J:697:GLU:OE1	1:J:697:GLU:N	2.29	0.62
1:P:697:GLU:N	1:P:697:GLU:OE1	2.28	0.62
2:K:283:ASN:OD1	2:K:284:LEU:N	2.27	0.62
3:O:1:MET:N	3:O:218:ASP:OD2	2.29	0.62
3:R:361:ASP:HB3	3:R:364:VAL:HG13	1.81	0.62
1:D:422:ILE:O	1:D:439:LYS:HB2	1.98	0.62
1:G:375:PHE:HD1	1:G:402:ILE:HD13	1.64	0.62
1:J:422:ILE:O	1:J:439:LYS:HB2	1.98	0.62
1:J:49:THR:O	1:J:49:THR:OG1	2.18	0.62
3:O:303:THR:HG22	3:O:304:HIS:H	1.64	0.62
1:J:271:ILE:O	1:J:289:SER:CB	2.47	0.62
1:J:503:GLY:O	1:J:504:THR:OG1	2.17	0.62
1:J:67:ASP:OD1	1:J:545:SER:OG	2.16	0.62
3:L:412:ARG:NH2	3:L:439:GLU:OE2	2.33	0.62
3:C:369:ALA:HB1	3:C:411:VAL:HG23	1.80	0.62
1:D:656:HIS:H	1:D:656:HIS:CD2	2.15	0.62
3:F:26:TYR:HB3	3:F:169:PRO:HB3	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:365:TRP:HB2	1:J:371:LYS:O	1.99	0.62
2:Q:503:SER:O	2:Q:507:ASN:ND2	2.30	0.62
1:A:454:GLN:HA	1:A:455:LYS:HE2	1.82	0.62
1:M:365:TRP:HB2	1:M:371:LYS:O	1.99	0.62
1:A:365:TRP:HB2	1:A:371:LYS:O	2.00	0.61
3:C:346:ILE:HD12	3:C:375:LYS:HD3	1.82	0.61
1:D:503:GLY:O	1:D:504:THR:OG1	2.16	0.61
3:I:26:TYR:HB3	3:I:169:PRO:HB3	1.82	0.61
1:P:479:HIS:NE2	1:P:491:SER:OG	2.27	0.61
2:E:274:ILE:HG23	2:E:282:ARG:HH22	1.65	0.61
1:G:365:TRP:HB2	1:G:371:LYS:O	2.00	0.61
1:G:656:HIS:CD2	1:G:656:HIS:H	2.15	0.61
3:I:412:ARG:NH2	3:I:439:GLU:OE2	2.33	0.61
1:J:454:GLN:HA	1:J:455:LYS:HE2	1.82	0.61
1:J:662:LEU:O	1:J:665:ASN:ND2	2.33	0.61
2:K:218:SER:O	2:K:218:SER:OG	2.18	0.61
3:L:303:THR:HG22	3:L:304:HIS:H	1.65	0.61
1:P:662:LEU:O	1:P:665:ASN:ND2	2.32	0.61
3:R:303:THR:HG22	3:R:304:HIS:H	1.65	0.61
1:M:321:LYS:HA	1:M:361:LYS:HD3	1.81	0.61
1:D:49:THR:O	1:D:49:THR:OG1	2.18	0.61
3:F:303:THR:HG22	3:F:304:HIS:H	1.65	0.61
3:O:412:ARG:NH2	3:O:439:GLU:OE2	2.33	0.61
2:E:212:VAL:O	2:E:216:GLU:HG2	2.00	0.61
1:D:174:TRP:HB3	3:F:198:LEU:HD23	1.82	0.61
3:F:250:LEU:HB2	3:F:270:PHE:HE2	1.66	0.61
1:G:454:GLN:HA	1:G:455:LYS:HE2	1.82	0.61
3:I:303:THR:HG22	3:I:304:HIS:H	1.66	0.61
1:P:448:THR:CG2	1:P:471:MET:H	2.14	0.61
1:G:269:PHE:HB2	1:G:300:LEU:HD11	1.80	0.61
1:G:662:LEU:O	1:G:665:ASN:ND2	2.33	0.61
3:I:361:ASP:HB3	3:I:364:VAL:HG13	1.82	0.61
2:N:418:PRO:HD2	3:O:233:TYR:OH	2.01	0.61
3:O:346:ILE:HD12	3:O:375:LYS:HD3	1.83	0.61
1:G:301:GLN:HG3	1:G:361:LYS:H	1.66	0.61
3:I:346:ILE:HD12	3:I:375:LYS:HD3	1.82	0.61
1:M:271:ILE:O	1:M:289:SER:CB	2.48	0.61
1:P:321:LYS:HA	1:P:361:LYS:HD3	1.81	0.61
2:E:418:PRO:HD2	3:F:233:TYR:OH	2.00	0.61
1:G:271:ILE:O	1:G:289:SER:CB	2.49	0.61
1:G:724:LEU:HD13	2:H:447:ALA:HB2	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:365:TRP:HB2	1:P:371:LYS:O	2.00	0.61
1:P:454:GLN:HA	1:P:455:LYS:HE2	1.82	0.61
2:Q:212:VAL:O	2:Q:216:GLU:HG2	2.00	0.61
3:F:361:ASP:HB3	3:F:364:VAL:HG13	1.82	0.61
3:I:250:LEU:HB2	3:I:270:PHE:HE2	1.66	0.61
1:M:454:GLN:HA	1:M:455:LYS:HE2	1.81	0.61
1:P:503:GLY:O	1:P:504:THR:OG1	2.17	0.61
1:D:662:LEU:O	1:D:665:ASN:ND2	2.33	0.61
2:E:309:TYR:O	2:E:313:THR:OG1	2.16	0.61
2:H:212:VAL:O	2:H:216:GLU:HG2	2.00	0.61
1:J:367:SER:HB2	1:J:369:PHE:HB2	1.83	0.61
3:L:359:MET:N	3:L:359:MET:SD	2.74	0.61
1:M:375:PHE:HD1	1:M:402:ILE:HD13	1.65	0.61
1:M:662:LEU:O	1:M:665:ASN:ND2	2.32	0.61
1:A:322:GLY:O	1:A:351:ILE:N	2.23	0.60
3:F:359:MET:N	3:F:359:MET:SD	2.74	0.60
3:F:346:ILE:HD12	3:F:375:LYS:HD3	1.83	0.60
1:G:697:GLU:N	1:G:697:GLU:OE1	2.28	0.60
3:C:26:TYR:HB3	3:C:169:PRO:HB3	1.83	0.60
3:C:412:ARG:NH2	3:C:439:GLU:OE2	2.33	0.60
1:D:448:THR:CG2	1:D:471:MET:H	2.14	0.60
1:D:724:LEU:HD13	2:E:447:ALA:HB2	1.83	0.60
3:L:346:ILE:HD12	3:L:375:LYS:HD3	1.83	0.60
3:R:346:ILE:HD12	3:R:375:LYS:HD3	1.83	0.60
2:H:218:SER:OG	2:H:218:SER:O	2.18	0.60
1:M:724:LEU:HD13	2:N:447:ALA:HB2	1.83	0.60
3:O:26:TYR:HB3	3:O:169:PRO:HB3	1.83	0.60
1:P:365:TRP:HB3	1:P:372:ILE:HG22	1.83	0.60
1:G:448:THR:CG2	1:G:471:MET:H	2.14	0.60
1:J:317:ILE:HG22	1:J:363:ILE:HD13	1.83	0.60
2:K:212:VAL:O	2:K:216:GLU:HG2	2.01	0.60
3:O:359:MET:N	3:O:359:MET:SD	2.74	0.60
1:P:367:SER:HB2	1:P:369:PHE:HB2	1.83	0.60
1:A:367:SER:HB2	1:A:369:PHE:HB2	1.83	0.60
1:D:271:ILE:O	1:D:289:SER:CB	2.48	0.60
1:G:503:GLY:O	1:G:504:THR:OG1	2.16	0.60
2:N:212:VAL:O	2:N:216:GLU:HG2	2.01	0.60
1:M:592:LEU:O	1:M:596:ILE:HG22	2.02	0.60
1:A:174:TRP:HB3	3:C:198:LEU:HD23	1.83	0.60
3:C:359:MET:N	3:C:359:MET:SD	2.74	0.60
3:L:361:ASP:HB3	3:L:364:VAL:HG13	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:418:PRO:HD2	3:R:233:TYR:OH	2.01	0.60
1:P:724:LEU:HD13	2:Q:447:ALA:HB2	1.84	0.60
3:R:250:LEU:HB2	3:R:270:PHE:HE2	1.66	0.60
1:A:375:PHE:HD1	1:A:402:ILE:HD13	1.65	0.60
1:A:448:THR:CG2	1:A:471:MET:H	2.15	0.60
1:D:375:PHE:HD1	1:D:402:ILE:HD13	1.66	0.60
1:D:592:LEU:O	1:D:596:ILE:HG22	2.02	0.60
3:L:421:LYS:HG3	3:L:422:GLY:H	1.67	0.60
1:M:367:SER:HB2	1:M:369:PHE:HB2	1.83	0.60
1:M:448:THR:CG2	1:M:471:MET:H	2.15	0.60
1:P:375:PHE:HD1	1:P:402:ILE:HD13	1.64	0.60
2:E:218:SER:OG	2:E:218:SER:O	2.19	0.60
2:K:366:TYR:CD1	3:L:215:THR:HG23	2.37	0.60
1:P:301:GLN:HG3	1:P:361:LYS:H	1.67	0.60
2:Q:103:LEU:HD21	2:Q:205:ILE:HG21	1.84	0.60
1:A:317:ILE:HG22	1:A:363:ILE:HD13	1.84	0.60
2:B:418:PRO:HD2	3:C:233:TYR:OH	2.02	0.60
3:F:421:LYS:HG3	3:F:422:GLY:H	1.66	0.60
1:G:448:THR:HG23	1:G:471:MET:H	1.65	0.60
3:L:26:TYR:HB3	3:L:169:PRO:HB3	1.82	0.60
2:N:366:TYR:CD1	3:O:215:THR:HG23	2.37	0.60
3:O:250:LEU:HB2	3:O:270:PHE:HE2	1.66	0.60
3:O:253:ILE:HA	3:O:256:GLU:HB3	1.84	0.60
3:C:236:PHE:O	3:C:240:ILE:HG22	2.02	0.59
3:C:361:ASP:HB3	3:C:364:VAL:HG13	1.82	0.59
1:G:185:GLN:HB3	1:G:247:ILE:HD13	1.84	0.59
3:I:421:LYS:HG3	3:I:422:GLY:H	1.67	0.59
1:J:185:GLN:HB3	1:J:247:ILE:HD13	1.84	0.59
1:A:56:ASP:OD1	1:A:554:ASN:ND2	2.35	0.59
1:D:367:SER:HB2	1:D:369:PHE:HB2	1.83	0.59
1:D:454:GLN:HA	1:D:455:LYS:HE2	1.82	0.59
1:G:317:ILE:HG22	1:G:363:ILE:HD13	1.83	0.59
1:G:49:THR:O	1:G:49:THR:OG1	2.18	0.59
1:P:56:ASP:OD1	1:P:554:ASN:ND2	2.35	0.59
1:A:592:LEU:O	1:A:596:ILE:HG22	2.02	0.59
2:E:103:LEU:HD21	2:E:205:ILE:HG21	1.84	0.59
1:A:724:LEU:HD13	2:B:447:ALA:HB2	1.84	0.59
3:C:421:LYS:HG3	3:C:422:GLY:H	1.66	0.59
1:D:301:GLN:HG3	1:D:361:LYS:H	1.67	0.59
1:G:407:ARG:HH22	1:G:411:LYS:HA	1.68	0.59
1:M:365:TRP:HB3	1:M:372:ILE:HG22	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:769:GLN:HA	1:P:772:ILE:HB	1.85	0.59
3:R:359:MET:SD	3:R:359:MET:N	2.74	0.59
3:C:250:LEU:HB2	3:C:270:PHE:HE2	1.66	0.59
3:C:253:ILE:HA	3:C:256:GLU:HB3	1.85	0.59
2:H:418:PRO:HD2	3:I:233:TYR:OH	2.02	0.59
3:I:359:MET:SD	3:I:359:MET:N	2.75	0.59
1:J:592:LEU:O	1:J:596:ILE:HG22	2.01	0.59
2:K:103:LEU:HD21	2:K:205:ILE:HG21	1.84	0.59
1:M:317:ILE:HG22	1:M:363:ILE:HD13	1.83	0.59
1:P:414:ILE:HB	1:P:425:GLY:O	2.03	0.59
1:P:665:ASN:N	1:P:665:ASN:OD1	2.34	0.59
3:R:26:TYR:HB3	3:R:169:PRO:HB3	1.84	0.59
1:G:367:SER:HB2	1:G:369:PHE:HB2	1.83	0.59
1:J:448:THR:CG2	1:J:471:MET:H	2.16	0.59
1:M:420:GLU:HA	1:M:442:LEU:O	2.03	0.59
3:O:421:LYS:HG3	3:O:422:GLY:H	1.66	0.59
2:B:212:VAL:O	2:B:216:GLU:HG2	2.02	0.59
1:D:448:THR:HG23	1:D:471:MET:H	1.67	0.59
1:D:665:ASN:N	1:D:665:ASN:OD1	2.35	0.59
1:G:365:TRP:HB3	1:G:372:ILE:HG22	1.83	0.59
1:M:301:GLN:HG3	1:M:361:LYS:H	1.68	0.59
1:P:448:THR:HG23	1:P:471:MET:H	1.67	0.59
1:P:592:LEU:O	1:P:596:ILE:HG22	2.03	0.59
1:A:448:THR:HG23	1:A:471:MET:H	1.68	0.59
1:D:365:TRP:HB3	1:D:372:ILE:HG22	1.85	0.59
1:J:534:VAL:HA	1:J:552:LEU:O	2.03	0.59
1:J:724:LEU:HD13	2:K:447:ALA:HB2	1.84	0.59
1:M:407:ARG:HH22	1:M:411:LYS:HA	1.68	0.59
1:A:49:THR:OG1	1:A:49:THR:O	2.18	0.59
1:D:382:GLU:OE2	1:D:432:PRO:HG2	2.03	0.59
2:H:288:GLU:HG3	2:H:297:ARG:HH12	1.68	0.59
1:J:301:GLN:HG3	1:J:361:LYS:H	1.68	0.59
1:M:448:THR:HG23	1:M:471:MET:H	1.67	0.59
1:P:382:GLU:OE2	1:P:432:PRO:HG2	2.03	0.59
1:A:301:GLN:HG3	1:A:361:LYS:H	1.68	0.59
1:A:414:ILE:HB	1:A:425:GLY:O	2.03	0.59
1:D:56:ASP:OD1	1:D:554:ASN:ND2	2.34	0.59
1:G:382:GLU:OE2	1:G:432:PRO:HG2	2.03	0.59
1:G:56:ASP:OD1	1:G:554:ASN:ND2	2.34	0.59
2:K:222:PHE:HA	2:K:492:ALA:HB1	1.85	0.59
3:L:253:ILE:HA	3:L:256:GLU:HB3	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:250:LEU:HB2	3:L:270:PHE:HE2	1.66	0.59
1:M:769:GLN:HA	1:M:772:ILE:HB	1.85	0.59
1:P:534:VAL:HA	1:P:552:LEU:O	2.03	0.59
2:Q:335:THR:HG21	2:Q:478:ARG:HG3	1.84	0.59
1:A:365:TRP:HB3	1:A:372:ILE:HG22	1.84	0.58
1:D:420:GLU:HA	1:D:442:LEU:O	2.03	0.58
1:G:420:GLU:HA	1:G:442:LEU:O	2.03	0.58
1:M:623:LEU:HG	1:M:678:LEU:HD12	1.84	0.58
1:A:484:ARG:HD2	1:A:488:LEU:HD12	1.85	0.58
1:M:534:VAL:HA	1:M:552:LEU:O	2.03	0.58
1:A:534:VAL:HA	1:A:552:LEU:O	2.04	0.58
2:H:274:ILE:HG23	2:H:282:ARG:HH22	1.68	0.58
2:H:335:THR:HG21	2:H:478:ARG:HG3	1.86	0.58
1:J:484:ARG:HD2	1:J:488:LEU:HD12	1.85	0.58
3:L:236:PHE:O	3:L:240:ILE:HG22	2.03	0.58
1:M:56:ASP:OD1	1:M:554:ASN:ND2	2.36	0.58
1:A:769:GLN:HA	1:A:772:ILE:HB	1.85	0.58
1:D:534:VAL:HA	1:D:552:LEU:O	2.03	0.58
1:D:769:GLN:HA	1:D:772:ILE:HB	1.85	0.58
2:E:288:GLU:HG3	2:E:297:ARG:HH12	1.68	0.58
2:E:335:THR:HG21	2:E:478:ARG:HG3	1.85	0.58
1:G:592:LEU:O	1:G:596:ILE:HG22	2.02	0.58
2:K:335:THR:HG21	2:K:478:ARG:HG3	1.86	0.58
2:Q:288:GLU:HG3	2:Q:297:ARG:HH12	1.68	0.58
3:R:426:VAL:HG12	3:R:427:PRO:HD3	1.86	0.58
1:G:534:VAL:HA	1:G:552:LEU:O	2.03	0.58
2:H:103:LEU:HD21	2:H:205:ILE:HG21	1.85	0.58
1:J:769:GLN:HA	1:J:772:ILE:HB	1.85	0.58
1:M:185:GLN:HB3	1:M:247:ILE:HD13	1.84	0.58
1:M:251:SER:HB3	1:M:411:LYS:HD2	1.86	0.58
1:P:174:TRP:HB3	3:R:198:LEU:HD23	1.86	0.58
1:P:407:ARG:HH22	1:P:411:LYS:HA	1.68	0.58
1:P:420:GLU:HA	1:P:442:LEU:O	2.04	0.58
3:R:253:ILE:HA	3:R:256:GLU:HB3	1.85	0.58
3:R:421:LYS:HG3	3:R:422:GLY:H	1.67	0.58
1:A:479:HIS:NE2	1:A:491:SER:OG	2.25	0.58
1:D:407:ARG:HH22	1:D:411:LYS:HA	1.69	0.58
2:E:222:PHE:HA	2:E:492:ALA:HB1	1.84	0.58
1:J:407:ARG:HH22	1:J:411:LYS:HA	1.69	0.58
3:O:236:PHE:O	3:O:240:ILE:HG22	2.03	0.58
1:A:185:GLN:HB3	1:A:247:ILE:HD13	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:152:LEU:HB3	2:E:154:LEU:HD22	1.86	0.58
2:E:162:ILE:HG22	2:E:226:LEU:HD21	1.85	0.58
2:E:366:TYR:CD1	3:F:215:THR:HG23	2.39	0.58
3:F:320:CYS:O	3:F:323:SER:N	2.37	0.58
2:H:222:PHE:HA	2:H:492:ALA:HB1	1.84	0.58
3:I:236:PHE:O	3:I:240:ILE:HG22	2.03	0.58
1:J:414:ILE:HB	1:J:425:GLY:O	2.04	0.58
1:M:414:ILE:HB	1:M:425:GLY:O	2.04	0.58
3:R:320:CYS:O	3:R:323:SER:N	2.37	0.58
1:A:407:ARG:HH22	1:A:411:LYS:HA	1.68	0.58
1:D:484:ARG:HD2	1:D:488:LEU:HD12	1.85	0.58
1:G:484:ARG:HD2	1:G:488:LEU:HD12	1.85	0.58
2:H:366:TYR:CD1	3:I:215:THR:HG23	2.39	0.58
1:J:320:ILE:HG13	1:J:323:ASN:OD1	2.04	0.58
1:J:448:THR:HG23	1:J:471:MET:H	1.69	0.58
1:M:382:GLU:OE2	1:M:432:PRO:HG2	2.03	0.58
1:A:382:GLU:OE2	1:A:432:PRO:HG2	2.03	0.58
2:B:103:LEU:HD21	2:B:205:ILE:HG21	1.84	0.58
1:G:59:ILE:HG22	1:G:60:VAL:H	1.69	0.58
1:G:665:ASN:N	1:G:665:ASN:OD1	2.34	0.58
1:J:174:TRP:HB3	3:L:198:LEU:HD23	1.85	0.58
1:J:420:GLU:HA	1:J:442:LEU:O	2.04	0.58
3:F:426:VAL:HG12	3:F:427:PRO:HD3	1.86	0.58
1:G:320:ILE:HG13	1:G:323:ASN:OD1	2.04	0.58
1:M:665:ASN:OD1	1:M:665:ASN:N	2.34	0.58
1:A:420:GLU:HA	1:A:442:LEU:O	2.03	0.57
2:B:222:PHE:HA	2:B:492:ALA:HB1	1.86	0.57
1:G:479:HIS:NE2	1:G:491:SER:OG	2.25	0.57
1:G:769:GLN:HA	1:G:772:ILE:HB	1.84	0.57
2:H:152:LEU:HB3	2:H:154:LEU:HD22	1.86	0.57
1:G:174:TRP:HB3	3:I:198:LEU:HD23	1.85	0.57
1:J:382:GLU:OE2	1:J:432:PRO:HG2	2.04	0.57
2:K:288:GLU:HG3	2:K:297:ARG:HH12	1.69	0.57
2:N:222:PHE:HA	2:N:492:ALA:HB1	1.85	0.57
1:M:573:GLU:HB2	2:N:499:LYS:HZ3	1.69	0.57
1:P:185:GLN:HB3	1:P:247:ILE:HD13	1.84	0.57
2:Q:152:LEU:HB3	2:Q:154:LEU:HD22	1.86	0.57
2:Q:309:TYR:O	2:Q:313:THR:OG1	2.16	0.57
1:A:404:ASP:OD1	1:A:405:TYR:N	2.37	0.57
1:A:725:VAL:HG21	2:B:446:TYR:CD1	2.39	0.57
2:B:274:ILE:HG23	2:B:282:ARG:HH22	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:725:VAL:HG21	2:E:446:TYR:CD1	2.38	0.57
1:M:322:GLY:O	1:M:351:ILE:N	2.25	0.57
1:M:49:THR:OG1	1:M:49:THR:O	2.18	0.57
1:P:49:THR:O	1:P:49:THR:OG1	2.18	0.57
1:P:67:ASP:OD1	1:P:545:SER:OG	2.16	0.57
2:B:335:THR:HG21	2:B:478:ARG:HG3	1.86	0.57
1:D:185:GLN:HB3	1:D:247:ILE:HD13	1.84	0.57
1:D:414:ILE:HB	1:D:425:GLY:O	2.03	0.57
3:F:253:ILE:HA	3:F:256:GLU:HB3	1.86	0.57
1:J:623:LEU:HG	1:J:678:LEU:HD12	1.85	0.57
2:N:162:ILE:HG22	2:N:226:LEU:HD21	1.86	0.57
1:P:317:ILE:HG22	1:P:363:ILE:HD13	1.84	0.57
1:P:251:SER:HB3	1:P:411:LYS:HD2	1.86	0.57
1:P:420:GLU:HG2	1:P:441:ASP:HB2	1.86	0.57
2:Q:274:ILE:HG23	2:Q:282:ARG:HH22	1.70	0.57
3:F:236:PHE:O	3:F:240:ILE:HG22	2.04	0.57
1:G:623:LEU:HG	1:G:678:LEU:HD12	1.85	0.57
3:I:157:MET:HG3	3:I:162:PHE:HB2	1.87	0.57
1:M:656:HIS:HB2	1:M:747:LEU:O	2.05	0.57
2:N:103:LEU:HD21	2:N:205:ILE:HG21	1.85	0.57
2:Q:222:PHE:HA	2:Q:492:ALA:HB1	1.84	0.57
3:R:157:MET:HG3	3:R:162:PHE:HB2	1.87	0.57
1:A:420:GLU:HG2	1:A:441:ASP:HB2	1.86	0.57
2:B:366:TYR:CD1	3:C:215:THR:HG23	2.40	0.57
1:G:631:SER:O	1:G:686:TYR:OH	2.22	0.57
3:I:253:ILE:HA	3:I:256:GLU:HB3	1.86	0.57
2:K:418:PRO:HD2	3:L:233:TYR:OH	2.04	0.57
2:N:288:GLU:HG3	2:N:297:ARG:HH12	1.69	0.57
3:O:323:SER:OG	3:O:324:MET:N	2.38	0.57
2:E:337:SER:HB2	2:E:448:LYS:HD3	1.87	0.57
3:F:157:MET:HG3	3:F:162:PHE:HB2	1.87	0.57
1:G:67:ASP:OD1	1:G:545:SER:OG	2.16	0.57
1:J:365:TRP:HB3	1:J:372:ILE:HG22	1.85	0.57
2:K:274:ILE:HG23	2:K:282:ARG:HH22	1.69	0.57
1:M:174:TRP:HB3	3:O:198:LEU:HD23	1.87	0.57
1:J:319:ASP:HB2	1:J:363:ILE:HG12	1.87	0.57
1:J:384:ASP:HB3	1:J:389:TRP:CD1	2.40	0.57
2:K:361:PRO:O	2:K:363:SER:N	2.38	0.57
1:M:59:ILE:HG22	1:M:60:VAL:H	1.69	0.57
2:N:335:THR:HG21	2:N:478:ARG:HG3	1.86	0.57
1:A:251:SER:HB3	1:A:411:LYS:HD2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:656:HIS:HB2	1:A:747:LEU:O	2.05	0.57
2:B:288:GLU:HG3	2:B:297:ARG:HH12	1.68	0.57
1:D:317:ILE:HG22	1:D:363:ILE:HD13	1.85	0.57
1:J:577:LEU:O	2:K:506:LYS:NZ	2.35	0.57
3:L:157:MET:HG3	3:L:162:PHE:HB2	1.86	0.57
1:P:484:ARG:HD2	1:P:488:LEU:HD12	1.86	0.57
1:G:656:HIS:HB2	1:G:747:LEU:O	2.05	0.57
2:H:337:SER:HB2	2:H:448:LYS:HD3	1.87	0.57
3:L:426:VAL:HG12	3:L:427:PRO:HD3	1.87	0.57
1:M:725:VAL:HG21	2:N:446:TYR:CD1	2.39	0.57
3:I:426:VAL:HG12	3:I:427:PRO:HD3	1.87	0.57
1:J:251:SER:HB3	1:J:411:LYS:HD2	1.86	0.57
3:L:323:SER:OG	3:L:324:MET:N	2.38	0.57
1:P:59:ILE:HG22	1:P:60:VAL:H	1.69	0.57
1:A:384:ASP:HB3	1:A:389:TRP:CD1	2.40	0.56
2:B:321:ASP:O	2:B:324:ARG:N	2.24	0.56
1:D:420:GLU:HG2	1:D:441:ASP:HB2	1.87	0.56
1:G:725:VAL:HG21	2:H:446:TYR:CD1	2.39	0.56
1:P:320:ILE:HG13	1:P:323:ASN:OD1	2.05	0.56
3:C:415:LEU:HD22	3:C:431:ILE:HG21	1.87	0.56
1:D:320:ILE:HG13	1:D:323:ASN:OD1	2.04	0.56
1:J:322:GLY:O	1:J:351:ILE:N	2.24	0.56
1:M:384:ASP:HB3	1:M:389:TRP:CD1	2.41	0.56
1:P:623:LEU:HG	1:P:678:LEU:HD12	1.85	0.56
1:D:204:ALA:HA	1:D:215:ASN:O	2.06	0.56
1:J:56:ASP:OD1	1:J:554:ASN:ND2	2.35	0.56
2:K:116:ILE:O	2:K:120:ILE:HG12	2.05	0.56
1:A:608:GLN:HA	1:A:611:ILE:HD12	1.87	0.56
3:C:426:VAL:HG12	3:C:427:PRO:HD3	1.87	0.56
1:G:251:SER:HB3	1:G:411:LYS:HD2	1.86	0.56
3:L:415:LEU:HD22	3:L:431:ILE:HG21	1.87	0.56
3:O:320:CYS:O	3:O:323:SER:N	2.37	0.56
1:P:656:HIS:HB2	1:P:747:LEU:O	2.05	0.56
1:A:320:ILE:HG13	1:A:323:ASN:OD1	2.06	0.56
2:B:361:PRO:O	2:B:363:SER:N	2.38	0.56
2:E:286:LEU:HD22	2:E:300:ASN:HB3	1.86	0.56
1:G:775:TRP:O	2:H:113:LYS:NZ	2.38	0.56
2:H:361:PRO:O	2:H:363:SER:N	2.39	0.56
3:I:320:CYS:O	3:I:323:SER:N	2.38	0.56
1:J:665:ASN:OD1	1:J:665:ASN:N	2.34	0.56
1:J:656:HIS:HB2	1:J:747:LEU:O	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:152:LEU:HB3	2:K:154:LEU:HD22	1.86	0.56
1:M:319:ASP:HB2	1:M:363:ILE:HG12	1.87	0.56
1:M:422:ILE:HG12	1:M:442:LEU:CD1	2.36	0.56
1:M:484:ARG:HD2	1:M:488:LEU:HD12	1.86	0.56
1:M:608:GLN:HA	1:M:611:ILE:HD12	1.88	0.56
1:M:67:ASP:OD1	1:M:545:SER:OG	2.15	0.56
2:Q:286:LEU:HD22	2:Q:300:ASN:HB3	1.86	0.56
2:Q:337:SER:HB2	2:Q:448:LYS:HD3	1.87	0.56
3:F:323:SER:OG	3:F:324:MET:N	2.38	0.56
2:H:286:LEU:HD22	2:H:300:ASN:HB3	1.87	0.56
1:J:659:LEU:HD12	1:J:742:TRP:CD1	2.40	0.56
1:M:775:TRP:O	2:N:113:LYS:NZ	2.38	0.56
2:N:337:SER:HB2	2:N:448:LYS:HD3	1.86	0.56
3:O:426:VAL:HG12	3:O:427:PRO:HD3	1.87	0.56
1:A:665:ASN:N	1:A:665:ASN:OD1	2.34	0.56
2:B:162:ILE:HG22	2:B:226:LEU:HD21	1.87	0.56
1:D:656:HIS:HB2	1:D:747:LEU:O	2.05	0.56
1:G:414:ILE:HB	1:G:425:GLY:O	2.05	0.56
1:G:422:ILE:HG12	1:G:442:LEU:CD1	2.36	0.56
1:J:59:ILE:HG22	1:J:60:VAL:H	1.69	0.56
2:N:286:LEU:HD22	2:N:300:ASN:HB3	1.87	0.56
2:N:361:PRO:O	2:N:363:SER:N	2.38	0.56
3:O:157:MET:HG3	3:O:162:PHE:HB2	1.87	0.56
1:D:384:ASP:HB3	1:D:389:TRP:CD1	2.40	0.56
1:G:384:ASP:HB3	1:G:389:TRP:CD1	2.41	0.56
2:H:104:PHE:HZ	2:H:156:LEU:HB2	1.70	0.56
1:J:420:GLU:HG2	1:J:441:ASP:HB2	1.86	0.56
2:K:227:TYR:O	2:K:230:ILE:HG13	2.05	0.56
2:N:152:LEU:HB3	2:N:154:LEU:HD22	1.86	0.56
1:P:384:ASP:HB3	1:P:389:TRP:CD1	2.40	0.56
2:Q:366:TYR:CD1	3:R:215:THR:HG23	2.40	0.56
3:R:415:LEU:HD22	3:R:431:ILE:HG21	1.87	0.56
1:A:623:LEU:HG	1:A:678:LEU:HD12	1.86	0.56
1:D:608:GLN:HA	1:D:611:ILE:HD12	1.87	0.56
1:G:608:GLN:HA	1:G:611:ILE:HD12	1.88	0.56
2:H:227:TYR:O	2:H:230:ILE:HG13	2.06	0.56
2:N:309:TYR:O	2:N:313:THR:OG1	2.13	0.56
2:Q:361:PRO:O	2:Q:363:SER:N	2.38	0.56
3:R:236:PHE:O	3:R:240:ILE:HG22	2.05	0.56
2:B:286:LEU:HD22	2:B:300:ASN:HB3	1.86	0.56
3:C:157:MET:HG3	3:C:162:PHE:HB2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:420:GLU:HG2	1:G:441:ASP:HB2	1.87	0.56
1:M:320:ILE:HG13	1:M:323:ASN:OD1	2.05	0.56
1:M:420:GLU:HG2	1:M:441:ASP:HB2	1.86	0.56
1:P:608:GLN:HA	1:P:611:ILE:HD12	1.88	0.56
2:Q:116:ILE:O	2:Q:120:ILE:HG12	2.06	0.56
1:A:319:ASP:HB2	1:A:363:ILE:HG12	1.87	0.56
1:D:59:ILE:HG22	1:D:60:VAL:H	1.71	0.56
1:D:623:LEU:HG	1:D:678:LEU:HD12	1.87	0.56
2:H:116:ILE:O	2:H:120:ILE:HG12	2.06	0.56
2:K:286:LEU:HD22	2:K:300:ASN:HB3	1.87	0.56
1:J:725:VAL:HG21	2:K:446:TYR:CD1	2.40	0.56
2:Q:162:ILE:HG22	2:Q:226:LEU:HD21	1.88	0.56
2:B:227:TYR:O	2:B:230:ILE:HG13	2.07	0.55
3:C:320:CYS:O	3:C:323:SER:N	2.36	0.55
3:F:415:LEU:HD22	3:F:431:ILE:HG21	1.87	0.55
1:G:715:TYR:CE1	1:G:733:THR:HG23	2.41	0.55
1:J:422:ILE:HG12	1:J:442:LEU:CD1	2.36	0.55
2:K:337:SER:HB2	2:K:448:LYS:HD3	1.87	0.55
2:N:495:LYS:HE2	2:N:499:LYS:HZ1	1.70	0.55
1:P:725:VAL:HG21	2:Q:446:TYR:CD1	2.40	0.55
1:A:532:GLU:HB2	1:A:554:ASN:HB3	1.89	0.55
2:B:152:LEU:HB3	2:B:154:LEU:HD22	1.87	0.55
1:J:775:TRP:HE1	1:J:778:ASP:HA	1.71	0.55
1:M:442:LEU:N	1:M:442:LEU:HD13	2.22	0.55
2:N:211:TYR:O	2:N:214:ILE:HG22	2.07	0.55
2:N:218:SER:OG	2:N:218:SER:O	2.19	0.55
3:O:361:ASP:O	3:O:364:VAL:HG22	2.07	0.55
3:R:361:ASP:O	3:R:364:VAL:HG22	2.07	0.55
2:B:116:ILE:O	2:B:120:ILE:HG12	2.05	0.55
2:B:441:ASP:O	2:B:445:ARG:HG2	2.07	0.55
2:E:361:PRO:O	2:E:363:SER:N	2.40	0.55
1:J:391:THR:HG23	3:L:149:LYS:HG2	1.87	0.55
1:J:608:GLN:HA	1:J:611:ILE:HD12	1.87	0.55
2:K:162:ILE:HG22	2:K:226:LEU:HD21	1.87	0.55
3:L:320:CYS:O	3:L:323:SER:N	2.37	0.55
1:P:319:ASP:HB2	1:P:363:ILE:HG12	1.87	0.55
1:A:204:ALA:HA	1:A:215:ASN:O	2.06	0.55
2:E:211:TYR:O	2:E:214:ILE:HG22	2.06	0.55
3:I:415:LEU:HD22	3:I:431:ILE:HG21	1.87	0.55
1:J:442:LEU:HD13	1:J:442:LEU:N	2.22	0.55
1:A:422:ILE:HG12	1:A:442:LEU:CD1	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:442:LEU:HD13	1:A:442:LEU:N	2.22	0.55
2:B:211:TYR:O	2:B:214:ILE:HG22	2.06	0.55
3:F:361:ASP:O	3:F:364:VAL:HG22	2.07	0.55
3:L:361:ASP:O	3:L:364:VAL:HG22	2.06	0.55
1:M:659:LEU:HD12	1:M:742:TRP:CD1	2.42	0.55
2:Q:211:TYR:O	2:Q:214:ILE:HG22	2.07	0.55
2:Q:362:THR:O	2:Q:365:ASP:HB2	2.07	0.55
2:K:321:ASP:O	2:K:324:ARG:N	2.24	0.55
2:Q:104:PHE:HZ	2:Q:156:LEU:HB2	1.70	0.55
1:A:659:LEU:HD12	1:A:742:TRP:CD1	2.42	0.55
2:B:337:SER:HB2	2:B:448:LYS:HD3	1.87	0.55
2:B:318:LEU:HB3	2:B:476:ILE:HD12	1.89	0.55
1:D:251:SER:HB3	1:D:411:LYS:HD2	1.87	0.55
1:D:384:ASP:OD2	1:D:387:ASN:HB2	2.07	0.55
1:D:422:ILE:HG12	1:D:442:LEU:CD1	2.36	0.55
2:E:116:ILE:O	2:E:120:ILE:HG12	2.06	0.55
1:G:204:ALA:HA	1:G:215:ASN:O	2.06	0.55
1:G:442:LEU:HD13	1:G:442:LEU:N	2.22	0.55
1:J:715:TYR:CE1	1:J:733:THR:HG23	2.42	0.55
3:R:323:SER:OG	3:R:324:MET:N	2.38	0.55
1:A:59:ILE:HG22	1:A:60:VAL:H	1.70	0.55
3:F:171:ARG:O	3:F:174:GLU:HB3	2.07	0.55
1:M:473:HIS:O	1:M:473:HIS:ND1	2.40	0.55
1:P:442:LEU:N	1:P:442:LEU:HD13	2.22	0.55
1:A:711:LEU:HD21	1:A:741:ILE:HD13	1.89	0.55
1:D:442:LEU:HD13	1:D:442:LEU:N	2.22	0.55
2:E:362:THR:O	2:E:365:ASP:HB2	2.07	0.55
1:G:532:GLU:HB2	1:G:554:ASN:HB3	1.89	0.55
2:K:318:LEU:HB3	2:K:476:ILE:HD12	1.89	0.55
1:D:775:TRP:O	2:E:113:LYS:NZ	2.39	0.55
2:H:162:ILE:HG22	2:H:226:LEU:HD21	1.88	0.55
3:I:361:ASP:O	3:I:364:VAL:HG22	2.07	0.55
1:J:404:ASP:OD1	1:J:405:TYR:N	2.39	0.55
2:N:321:ASP:O	2:N:324:ARG:N	2.24	0.55
3:O:415:LEU:HD22	3:O:431:ILE:HG21	1.88	0.55
2:E:198:ILE:HG21	2:E:389:GLN:HA	1.89	0.54
1:G:711:LEU:HD21	1:G:741:ILE:HD13	1.89	0.54
2:H:211:TYR:O	2:H:214:ILE:HG22	2.07	0.54
2:K:211:TYR:O	2:K:214:ILE:HG22	2.07	0.54
2:N:362:THR:O	2:N:365:ASP:HB2	2.07	0.54
3:R:171:ARG:O	3:R:174:GLU:HB3	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:384:ASP:OD2	1:A:387:ASN:HB2	2.07	0.54
2:B:362:THR:O	2:B:365:ASP:HB2	2.06	0.54
1:D:532:GLU:HB2	1:D:554:ASN:HB3	1.89	0.54
1:J:204:ALA:HA	1:J:215:ASN:O	2.07	0.54
1:J:631:SER:O	1:J:686:TYR:OH	2.26	0.54
2:K:257:VAL:HG13	2:K:262:LEU:HB2	1.88	0.54
2:K:198:ILE:HG21	2:K:389:GLN:HA	1.89	0.54
2:N:274:ILE:HG23	2:N:282:ARG:HH22	1.72	0.54
1:P:532:GLU:HB2	1:P:554:ASN:HB3	1.88	0.54
1:P:659:LEU:HD12	1:P:742:TRP:CD1	2.42	0.54
2:Q:227:TYR:O	2:Q:230:ILE:HG13	2.06	0.54
1:A:715:TYR:CE1	1:A:733:THR:HG23	2.42	0.54
1:A:775:TRP:HE1	1:A:778:ASP:HA	1.72	0.54
2:B:218:SER:OG	2:B:218:SER:O	2.18	0.54
3:C:361:ASP:O	3:C:364:VAL:HG22	2.07	0.54
2:E:441:ASP:O	2:E:445:ARG:HG2	2.07	0.54
1:G:384:ASP:OD2	1:G:387:ASN:HB2	2.07	0.54
2:H:441:ASP:O	2:H:445:ARG:HG2	2.07	0.54
1:M:204:ALA:HA	1:M:215:ASN:O	2.07	0.54
1:M:384:ASP:OD2	1:M:387:ASN:HB2	2.07	0.54
3:C:323:SER:OG	3:C:324:MET:N	2.38	0.54
1:D:414:ILE:HB	1:D:425:GLY:C	2.27	0.54
2:E:104:PHE:HZ	2:E:156:LEU:HB2	1.71	0.54
1:G:391:THR:HG23	3:I:149:LYS:HG2	1.89	0.54
1:G:414:ILE:HB	1:G:425:GLY:C	2.28	0.54
1:G:775:TRP:HE1	1:G:778:ASP:HA	1.72	0.54
1:J:532:GLU:HB2	1:J:554:ASN:HB3	1.89	0.54
2:K:441:ASP:O	2:K:445:ARG:HG2	2.08	0.54
3:O:171:ARG:O	3:O:174:GLU:HB3	2.07	0.54
1:P:399:TRP:O	1:P:419:ARG:NH2	2.40	0.54
1:D:319:ASP:HB2	1:D:363:ILE:HG12	1.89	0.54
1:D:775:TRP:HE1	1:D:778:ASP:HA	1.72	0.54
1:G:498:LEU:O	1:G:499:GLU:HG3	2.08	0.54
3:I:171:ARG:O	3:I:174:GLU:HB3	2.08	0.54
1:M:414:ILE:HB	1:M:425:GLY:C	2.28	0.54
1:M:532:GLU:HB2	1:M:554:ASN:HB3	1.89	0.54
2:N:318:LEU:HB3	2:N:476:ILE:HD12	1.89	0.54
1:P:422:ILE:HG12	1:P:442:LEU:CD1	2.37	0.54
1:P:715:TYR:CE1	1:P:733:THR:HG23	2.42	0.54
1:P:775:TRP:HE1	1:P:778:ASP:HA	1.71	0.54
2:B:104:PHE:HZ	2:B:156:LEU:HB2	1.71	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:495:LYS:HE2	2:E:499:LYS:HZ1	1.72	0.54
1:G:462:ILE:HB	1:G:483:HIS:HB3	1.89	0.54
1:M:599:LYS:HE3	2:N:272:GLN:HE22	1.71	0.54
2:N:116:ILE:O	2:N:120:ILE:HG12	2.06	0.54
2:N:104:PHE:HZ	2:N:156:LEU:HB2	1.71	0.54
2:N:227:TYR:O	2:N:230:ILE:HG13	2.06	0.54
2:Q:257:VAL:HG13	2:Q:262:LEU:HB2	1.90	0.54
1:A:675:PHE:CZ	1:A:742:TRP:HZ3	2.26	0.54
3:C:171:ARG:O	3:C:174:GLU:HB3	2.06	0.54
3:C:350:SER:HA	3:C:353:VAL:HB	1.90	0.54
2:E:103:LEU:HD21	2:E:205:ILE:HD13	1.89	0.54
1:G:404:ASP:OD1	1:G:405:TYR:N	2.38	0.54
1:J:408:ILE:HD12	1:J:464:LEU:HD13	1.90	0.54
1:M:391:THR:HG23	3:O:149:LYS:HG2	1.88	0.54
3:O:305:THR:HB	3:O:308:PHE:HE1	1.73	0.54
3:R:350:SER:HA	3:R:353:VAL:HB	1.90	0.54
1:A:391:THR:HG23	3:C:149:LYS:HG2	1.89	0.54
1:A:399:TRP:O	1:A:419:ARG:NH2	2.41	0.54
1:A:631:SER:O	1:A:686:TYR:OH	2.25	0.54
1:D:715:TYR:CE1	1:D:733:THR:HG23	2.43	0.54
1:G:319:ASP:HB2	1:G:363:ILE:HG12	1.88	0.54
2:H:509:CYS:O	2:H:513:MET:HB2	2.08	0.54
1:J:301:GLN:N	1:J:319:ASP:O	2.40	0.54
1:J:389:TRP:CH2	3:L:147:GLN:HA	2.43	0.54
2:K:509:CYS:O	2:K:513:MET:HB2	2.08	0.54
1:M:675:PHE:CZ	1:M:742:TRP:HZ3	2.25	0.54
1:M:715:TYR:CE1	1:M:733:THR:HG23	2.42	0.54
3:R:83:HIS:O	3:R:85:ARG:N	2.41	0.54
2:B:409:ALA:O	2:B:413:LEU:CB	2.52	0.54
1:G:659:LEU:HD12	1:G:742:TRP:CD1	2.42	0.54
2:H:103:LEU:HD21	2:H:205:ILE:HD13	1.90	0.54
1:J:254:ILE:HG23	1:J:256:ARG:H	1.73	0.54
1:J:775:TRP:O	2:K:113:LYS:NZ	2.40	0.54
3:L:217:THR:HG22	3:L:239:LEU:HD21	1.88	0.54
2:N:441:ASP:O	2:N:445:ARG:HG2	2.07	0.54
1:P:204:ALA:HA	1:P:215:ASN:O	2.07	0.54
1:P:254:ILE:HG23	1:P:256:ARG:H	1.72	0.54
2:Q:509:CYS:O	2:Q:513:MET:HB2	2.08	0.54
1:A:254:ILE:HG23	1:A:256:ARG:H	1.72	0.54
3:C:305:THR:HB	3:C:308:PHE:HE1	1.73	0.54
1:D:404:ASP:OD1	1:D:405:TYR:N	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:301:GLN:N	1:G:319:ASP:O	2.41	0.54
1:M:733:THR:HA	1:M:736:ILE:HG22	1.90	0.54
2:N:103:LEU:HD21	2:N:205:ILE:HD13	1.90	0.54
2:Q:318:LEU:HB3	2:Q:476:ILE:HD12	1.89	0.54
2:B:309:TYR:O	2:B:313:THR:OG1	2.16	0.53
1:D:711:LEU:HD21	1:D:741:ILE:HD13	1.90	0.53
2:H:318:LEU:HB3	2:H:476:ILE:HD12	1.89	0.53
1:J:462:ILE:HB	1:J:483:HIS:HB3	1.89	0.53
3:L:171:ARG:O	3:L:174:GLU:HB3	2.07	0.53
3:O:350:SER:HA	3:O:353:VAL:HB	1.90	0.53
1:A:330:PRO:HG3	1:A:342:GLN:CG	2.38	0.53
3:I:305:THR:HB	3:I:308:PHE:HE1	1.73	0.53
1:J:414:ILE:HB	1:J:425:GLY:C	2.27	0.53
1:J:498:LEU:O	1:J:499:GLU:HG3	2.09	0.53
1:J:722:TRP:CD1	2:K:264:PRO:HD3	2.43	0.53
1:M:301:GLN:N	1:M:319:ASP:O	2.41	0.53
1:M:775:TRP:HE1	1:M:778:ASP:HA	1.71	0.53
2:N:257:VAL:HG13	2:N:262:LEU:HB2	1.90	0.53
2:N:333:SER:HA	2:N:336:GLU:HG2	1.91	0.53
2:N:505:ILE:HA	2:N:508:ALA:HB3	1.90	0.53
3:O:83:HIS:O	3:O:85:ARG:N	2.41	0.53
1:P:414:ILE:HB	1:P:425:GLY:C	2.28	0.53
1:P:711:LEU:HD21	1:P:741:ILE:HD13	1.89	0.53
1:P:775:TRP:O	2:Q:113:LYS:NZ	2.41	0.53
3:R:217:THR:HG22	3:R:239:LEU:HD21	1.90	0.53
1:A:301:GLN:N	1:A:319:ASP:O	2.42	0.53
2:B:101:LYS:O	2:B:105:LEU:HG	2.09	0.53
1:D:292:LEU:HD11	1:D:343:LEU:HG	1.90	0.53
1:D:659:LEU:HD12	1:D:742:TRP:CD1	2.42	0.53
1:D:389:TRP:CH2	3:F:147:GLN:HA	2.43	0.53
1:G:675:PHE:CZ	1:G:742:TRP:HZ3	2.25	0.53
1:J:711:LEU:HD21	1:J:741:ILE:HD13	1.89	0.53
2:K:362:THR:O	2:K:365:ASP:HB2	2.07	0.53
1:P:301:GLN:N	1:P:319:ASP:O	2.41	0.53
1:P:675:PHE:CZ	1:P:742:TRP:HZ3	2.25	0.53
2:Q:333:SER:HA	2:Q:336:GLU:HG2	1.90	0.53
2:Q:441:ASP:O	2:Q:445:ARG:HG2	2.08	0.53
1:P:391:THR:HG23	3:R:149:LYS:HG2	1.90	0.53
1:A:462:ILE:HB	1:A:483:HIS:HB3	1.89	0.53
1:A:408:ILE:HD12	1:A:464:LEU:HD13	1.90	0.53
1:D:254:ILE:HG23	1:D:256:ARG:H	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:350:SER:HA	3:F:353:VAL:HB	1.90	0.53
2:H:495:LYS:HE2	2:H:499:LYS:HZ1	1.73	0.53
1:J:215:ASN:ND2	1:J:235:SER:HB3	2.24	0.53
2:K:333:SER:HA	2:K:336:GLU:HG2	1.90	0.53
1:M:404:ASP:OD1	1:M:405:TYR:N	2.37	0.53
1:P:384:ASP:OD2	1:P:387:ASN:HB2	2.08	0.53
1:P:631:SER:O	1:P:686:TYR:OH	2.26	0.53
3:C:83:HIS:O	3:C:85:ARG:N	2.42	0.53
2:E:333:SER:HA	2:E:336:GLU:HG2	1.90	0.53
2:E:318:LEU:HB3	2:E:476:ILE:HD12	1.89	0.53
1:J:659:LEU:HD12	1:J:742:TRP:NE1	2.24	0.53
3:O:217:THR:HG22	3:O:239:LEU:HD21	1.89	0.53
1:A:414:ILE:HB	1:A:425:GLY:C	2.28	0.53
1:A:733:THR:HA	1:A:736:ILE:HG22	1.91	0.53
1:A:389:TRP:CH2	3:C:147:GLN:HA	2.44	0.53
1:D:675:PHE:CZ	1:D:742:TRP:HZ3	2.26	0.53
1:D:631:SER:O	1:D:686:TYR:OH	2.26	0.53
3:F:305:THR:HB	3:F:308:PHE:HE1	1.73	0.53
1:G:733:THR:HA	1:G:736:ILE:HG22	1.90	0.53
1:G:653:SER:H	1:G:749:LYS:HB3	1.74	0.53
3:I:323:SER:OG	3:I:324:MET:N	2.38	0.53
1:J:384:ASP:OD2	1:J:387:ASN:HB2	2.08	0.53
3:L:83:HIS:O	3:L:85:ARG:N	2.42	0.53
2:N:198:ILE:HG21	2:N:389:GLN:HA	1.91	0.53
1:P:473:HIS:O	1:P:473:HIS:ND1	2.42	0.53
3:R:305:THR:HB	3:R:308:PHE:HE1	1.73	0.53
1:A:292:LEU:HD11	1:A:343:LEU:HG	1.90	0.53
1:A:659:LEU:HD12	1:A:742:TRP:NE1	2.24	0.53
1:D:399:TRP:O	1:D:419:ARG:NH2	2.41	0.53
2:E:227:TYR:O	2:E:230:ILE:HG13	2.07	0.53
2:H:362:THR:O	2:H:365:ASP:HB2	2.08	0.53
2:K:505:ILE:HA	2:K:508:ALA:HB3	1.91	0.53
1:M:389:TRP:CH2	3:O:147:GLN:HA	2.44	0.53
1:P:498:LEU:O	1:P:499:GLU:HG3	2.09	0.53
2:Q:103:LEU:HD21	2:Q:205:ILE:HD13	1.90	0.53
1:A:215:ASN:ND2	1:A:235:SER:HB3	2.24	0.53
1:A:775:TRP:O	2:B:113:LYS:NZ	2.39	0.53
3:C:217:THR:HG22	3:C:239:LEU:HD21	1.91	0.53
1:D:473:HIS:O	1:D:473:HIS:ND1	2.41	0.53
1:G:254:ILE:HG23	1:G:256:ARG:H	1.74	0.53
1:G:599:LYS:HE3	2:H:272:GLN:HE22	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:333:SER:HA	2:H:336:GLU:HG2	1.90	0.53
3:I:83:HIS:O	3:I:85:ARG:N	2.42	0.53
3:L:305:THR:HB	3:L:308:PHE:HE1	1.73	0.53
3:L:350:SER:HA	3:L:353:VAL:HB	1.90	0.53
2:E:509:CYS:O	2:E:513:MET:HB2	2.08	0.53
3:F:83:HIS:O	3:F:85:ARG:N	2.42	0.53
3:I:350:SER:HA	3:I:353:VAL:HB	1.90	0.53
1:J:454:GLN:HE22	1:J:536:ASP:H	1.57	0.53
2:K:101:LYS:O	2:K:105:LEU:HG	2.09	0.53
2:K:309:TYR:O	2:K:313:THR:OG1	2.17	0.53
1:M:330:PRO:HG3	1:M:342:GLN:CG	2.39	0.53
1:M:498:LEU:O	1:M:499:GLU:HG3	2.07	0.53
2:N:101:LYS:O	2:N:105:LEU:HG	2.08	0.53
2:N:509:CYS:O	2:N:513:MET:HB2	2.08	0.53
1:P:292:LEU:HD11	1:P:343:LEU:HG	1.91	0.53
2:B:333:SER:HA	2:B:336:GLU:HG2	1.91	0.53
1:D:215:ASN:ND2	1:D:235:SER:HB3	2.24	0.53
1:D:408:ILE:HG12	1:D:408:ILE:O	2.09	0.53
1:D:733:THR:HA	1:D:736:ILE:HG22	1.91	0.53
2:H:505:ILE:HA	2:H:508:ALA:HB3	1.91	0.53
3:L:177:LEU:HD22	3:L:185:LYS:HG2	1.91	0.53
1:M:254:ILE:HG23	1:M:256:ARG:H	1.74	0.53
1:M:462:ILE:HB	1:M:483:HIS:HB3	1.89	0.53
1:M:653:SER:H	1:M:749:LYS:HB3	1.74	0.53
1:P:215:ASN:ND2	1:P:235:SER:HB3	2.24	0.53
1:P:292:LEU:N	1:P:292:LEU:HD13	2.24	0.53
2:Q:495:LYS:HE2	2:Q:499:LYS:HZ1	1.74	0.53
2:Q:505:ILE:HA	2:Q:508:ALA:HB3	1.91	0.53
1:A:292:LEU:HD13	1:A:292:LEU:N	2.24	0.52
1:A:653:SER:H	1:A:749:LYS:HB3	1.74	0.52
2:B:505:ILE:HA	2:B:508:ALA:HB3	1.91	0.52
2:B:509:CYS:O	2:B:513:MET:HB2	2.08	0.52
1:D:653:SER:H	1:D:749:LYS:HB3	1.74	0.52
1:G:330:PRO:HG3	1:G:342:GLN:CG	2.38	0.52
1:J:653:SER:H	1:J:749:LYS:HB3	1.74	0.52
2:B:257:VAL:HG13	2:B:262:LEU:HB2	1.90	0.52
2:B:287:TRP:NE1	2:B:289:ARG:HB3	2.25	0.52
2:E:409:ALA:O	2:E:413:LEU:CB	2.52	0.52
1:J:292:LEU:HD13	1:J:292:LEU:N	2.25	0.52
1:J:675:PHE:CZ	1:J:742:TRP:HZ3	2.25	0.52
1:M:399:TRP:O	1:M:419:ARG:NH2	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:711:LEU:HD21	1:M:741:ILE:HD13	1.90	0.52
2:N:287:TRP:NE1	2:N:289:ARG:HB3	2.25	0.52
1:P:330:PRO:HG3	1:P:342:GLN:CG	2.39	0.52
1:P:389:TRP:CH2	3:R:147:GLN:HA	2.44	0.52
1:P:408:ILE:HG12	1:P:408:ILE:O	2.09	0.52
1:P:462:ILE:HB	1:P:483:HIS:HB3	1.90	0.52
2:E:274:ILE:HG23	2:E:282:ARG:NH2	2.25	0.52
2:E:505:ILE:HA	2:E:508:ALA:HB3	1.91	0.52
3:F:5:PRO:O	3:F:245:VAL:HA	2.09	0.52
1:G:215:ASN:ND2	1:G:235:SER:HB3	2.24	0.52
2:H:101:LYS:O	2:H:105:LEU:HG	2.09	0.52
1:G:389:TRP:CH2	3:I:147:GLN:HA	2.43	0.52
1:J:733:THR:HA	1:J:736:ILE:HG22	1.92	0.52
1:M:215:ASN:ND2	1:M:235:SER:HB3	2.24	0.52
1:M:292:LEU:N	1:M:292:LEU:HD13	2.24	0.52
1:M:659:LEU:HD12	1:M:742:TRP:NE1	2.24	0.52
2:Q:101:LYS:O	2:Q:105:LEU:HG	2.09	0.52
1:A:770:ASP:HB2	2:B:145:ASN:OD1	2.10	0.52
1:G:292:LEU:N	1:G:292:LEU:HD13	2.25	0.52
1:G:408:ILE:HB	1:G:453:VAL:HG21	1.92	0.52
1:G:659:LEU:HD12	1:G:742:TRP:NE1	2.24	0.52
2:H:287:TRP:NE1	2:H:289:ARG:HB3	2.25	0.52
1:J:330:PRO:HG3	1:J:342:GLN:CG	2.39	0.52
1:J:473:HIS:O	1:J:473:HIS:ND1	2.40	0.52
1:P:404:ASP:OD1	1:P:405:TYR:N	2.41	0.52
1:P:408:ILE:HD12	1:P:464:LEU:HD13	1.90	0.52
1:D:462:ILE:HB	1:D:483:HIS:HB3	1.90	0.52
3:F:217:THR:HG22	3:F:239:LEU:HD21	1.90	0.52
1:G:302:VAL:O	1:G:363:ILE:HD11	2.10	0.52
1:J:302:VAL:O	1:J:363:ILE:HD11	2.10	0.52
2:K:104:PHE:HZ	2:K:156:LEU:HB2	1.71	0.52
1:M:408:ILE:HG12	1:M:408:ILE:O	2.10	0.52
3:C:177:LEU:HD22	3:C:185:LYS:HG2	1.91	0.52
1:D:355:GLU:HB3	3:F:24:ILE:HG23	1.92	0.52
1:D:498:LEU:O	1:D:499:GLU:HG3	2.09	0.52
3:F:10:ASN:OD1	3:F:10:ASN:N	2.43	0.52
2:H:252:LEU:HD22	2:H:306:VAL:HG11	1.92	0.52
1:J:315:PHE:HB3	1:J:317:ILE:CD1	2.40	0.52
2:K:287:TRP:NE1	2:K:289:ARG:HB3	2.25	0.52
1:P:733:THR:HA	1:P:736:ILE:HG22	1.91	0.52
1:A:599:LYS:HE3	2:B:272:GLN:HE22	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:659:LEU:HD12	1:D:742:TRP:NE1	2.24	0.52
2:E:257:VAL:HG13	2:E:262:LEU:HB2	1.90	0.52
1:D:599:LYS:HE3	2:E:272:GLN:HE22	1.73	0.52
2:E:287:TRP:NE1	2:E:289:ARG:HB3	2.25	0.52
1:G:399:TRP:O	1:G:419:ARG:NH2	2.42	0.52
2:H:309:TYR:O	2:H:313:THR:OG1	2.16	0.52
1:P:408:ILE:HB	1:P:453:VAL:HG21	1.92	0.52
1:P:659:LEU:HD12	1:P:742:TRP:NE1	2.24	0.52
1:A:736:ILE:HD11	2:B:254:LEU:HD13	1.92	0.52
3:C:10:ASN:N	3:C:10:ASN:OD1	2.43	0.52
1:D:302:VAL:O	1:D:363:ILE:HD11	2.10	0.52
2:E:101:LYS:O	2:E:105:LEU:HG	2.10	0.52
1:G:292:LEU:CD1	1:G:343:LEU:HG	2.40	0.52
1:M:292:LEU:HD11	1:M:343:LEU:HG	1.91	0.52
1:A:315:PHE:HB3	1:A:317:ILE:CD1	2.40	0.52
2:E:344:THR:HG22	2:E:436:LEU:HD13	1.91	0.52
1:G:292:LEU:HD11	1:G:343:LEU:HG	1.91	0.52
1:G:315:PHE:HB3	1:G:317:ILE:CD1	2.40	0.52
1:G:607:VAL:HB	1:G:731:LEU:HD13	1.91	0.52
3:I:10:ASN:OD1	3:I:10:ASN:N	2.43	0.52
1:P:302:VAL:O	1:P:363:ILE:HD11	2.10	0.52
1:P:377:ARG:NH2	1:P:378:SER:OG	2.33	0.52
2:Q:218:SER:O	2:Q:218:SER:OG	2.21	0.52
1:P:599:LYS:HE3	2:Q:272:GLN:HE22	1.74	0.52
1:A:498:LEU:O	1:A:499:GLU:HG3	2.09	0.52
2:B:103:LEU:HD21	2:B:205:ILE:HD13	1.91	0.52
1:D:330:PRO:HG3	1:D:342:GLN:CG	2.39	0.52
1:J:232:ASN:O	1:J:232:ASN:ND2	2.44	0.52
2:K:495:LYS:HE2	2:K:499:LYS:HZ1	1.75	0.52
2:N:484:ALA:O	2:N:488:LEU:HG	2.10	0.52
1:P:292:LEU:CD1	1:P:343:LEU:HG	2.40	0.52
1:D:315:PHE:HB3	1:D:317:ILE:CD1	2.40	0.51
1:D:408:ILE:HD12	1:D:464:LEU:HD13	1.91	0.51
3:F:30:ARG:NE	3:F:168:ILE:HD12	2.25	0.51
1:G:667:ASP:N	1:G:667:ASP:OD1	2.43	0.51
3:I:217:THR:HG22	3:I:239:LEU:HD21	1.91	0.51
3:I:5:PRO:O	3:I:245:VAL:HA	2.10	0.51
3:L:30:ARG:NE	3:L:168:ILE:HD12	2.25	0.51
1:M:770:ASP:OD2	2:N:141:LEU:HG	2.10	0.51
1:P:232:ASN:O	1:P:232:ASN:ND2	2.44	0.51
1:P:315:PHE:HB3	1:P:317:ILE:CD1	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:161:ASN:O	3:C:164:LYS:HB2	2.10	0.51
3:C:5:PRO:O	3:C:245:VAL:HA	2.10	0.51
1:D:391:THR:HG23	3:F:149:LYS:HG2	1.92	0.51
1:J:599:LYS:HE3	2:K:272:GLN:HE22	1.75	0.51
1:A:292:LEU:CD1	1:A:343:LEU:HG	2.40	0.51
2:H:257:VAL:HG13	2:H:262:LEU:HB2	1.91	0.51
2:H:321:ASP:O	2:H:324:ARG:N	2.24	0.51
2:H:198:ILE:HG21	2:H:389:GLN:HA	1.92	0.51
3:I:30:ARG:NE	3:I:168:ILE:HD12	2.25	0.51
3:L:10:ASN:N	3:L:10:ASN:OD1	2.43	0.51
1:M:408:ILE:HB	1:M:453:VAL:HG21	1.92	0.51
2:Q:287:TRP:NE1	2:Q:289:ARG:HB3	2.25	0.51
1:D:232:ASN:ND2	1:D:232:ASN:O	2.44	0.51
1:D:292:LEU:CD1	1:D:343:LEU:HG	2.40	0.51
1:D:301:GLN:N	1:D:319:ASP:O	2.42	0.51
1:D:722:TRP:CD1	2:E:264:PRO:HD3	2.45	0.51
1:J:399:TRP:O	1:J:419:ARG:NH2	2.43	0.51
1:M:302:VAL:O	1:M:363:ILE:HD11	2.09	0.51
2:Q:198:ILE:HG21	2:Q:389:GLN:HA	1.93	0.51
1:A:302:VAL:O	1:A:363:ILE:HD11	2.10	0.51
1:A:473:HIS:O	1:A:473:HIS:ND1	2.41	0.51
1:J:408:ILE:HB	1:J:453:VAL:HG21	1.92	0.51
3:R:30:ARG:NE	3:R:168:ILE:HD12	2.24	0.51
1:A:232:ASN:ND2	1:A:232:ASN:O	2.43	0.51
2:B:198:ILE:HG21	2:B:389:GLN:HA	1.93	0.51
1:D:292:LEU:HD13	1:D:292:LEU:N	2.25	0.51
3:F:26:TYR:CB	3:F:169:PRO:HB3	2.41	0.51
3:I:26:TYR:CB	3:I:169:PRO:HB3	2.40	0.51
3:L:26:TYR:CB	3:L:169:PRO:HB3	2.41	0.51
1:M:454:GLN:HE22	1:M:536:ASP:H	1.59	0.51
1:P:653:SER:H	1:P:749:LYS:HB3	1.75	0.51
1:A:420:GLU:HA	1:A:442:LEU:HD22	1.92	0.51
3:C:26:TYR:CB	3:C:169:PRO:HB3	2.41	0.51
1:G:217:ALA:HB2	1:G:233:VAL:HA	1.92	0.51
1:G:603:ARG:O	1:G:607:VAL:HG23	2.11	0.51
3:I:161:ASN:O	3:I:164:LYS:HB2	2.11	0.51
3:L:213:ILE:HG12	3:L:242:ILE:HD13	1.93	0.51
1:M:217:ALA:HB2	1:M:233:VAL:HA	1.93	0.51
1:M:446:ASP:OD1	1:M:472:ARG:HD3	2.10	0.51
1:P:420:GLU:HA	1:P:442:LEU:HD22	1.93	0.51
1:P:474:LYS:CD	1:P:474:LYS:H	2.24	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:667:ASP:N	1:A:667:ASP:OD1	2.44	0.51
3:C:213:ILE:HG12	3:C:242:ILE:HD13	1.93	0.51
1:G:770:ASP:OD2	2:H:141:LEU:HG	2.11	0.51
3:I:213:ILE:HG12	3:I:242:ILE:HD13	1.93	0.51
2:K:103:LEU:HD21	2:K:205:ILE:HD13	1.91	0.51
2:K:344:THR:HG22	2:K:436:LEU:HD13	1.93	0.51
3:L:209:ARG:H	3:L:209:ARG:HD3	1.76	0.51
1:M:408:ILE:HD12	1:M:464:LEU:HD13	1.91	0.51
1:M:607:VAL:HB	1:M:731:LEU:HD13	1.92	0.51
1:M:631:SER:O	1:M:686:TYR:OH	2.28	0.51
3:O:273:TRP:O	3:O:277:ILE:HG22	2.11	0.51
3:O:75:GLN:HA	3:O:78:ARG:NE	2.25	0.51
2:Q:193:PHE:HD1	2:Q:219:ILE:HD11	1.75	0.51
1:A:217:ALA:HB2	1:A:233:VAL:HA	1.92	0.51
1:A:712:ASP:N	1:A:712:ASP:OD1	2.44	0.51
2:B:221:PRO:HA	2:B:225:GLN:HB2	1.93	0.51
3:C:273:TRP:O	3:C:277:ILE:HG22	2.11	0.51
1:D:667:ASP:N	1:D:667:ASP:OD1	2.44	0.51
2:N:409:ALA:O	2:N:413:LEU:CB	2.52	0.51
3:O:242:ILE:HG23	3:O:244:GLY:H	1.76	0.51
2:E:221:PRO:HA	2:E:225:GLN:HB2	1.93	0.51
1:G:712:ASP:N	1:G:712:ASP:OD1	2.44	0.51
1:G:767:PRO:O	1:G:771:ILE:HG12	2.11	0.51
1:J:603:ARG:O	1:J:607:VAL:HG23	2.11	0.51
2:K:109:GLN:OE1	2:K:137:TRP:NE1	2.40	0.51
1:M:315:PHE:HB3	1:M:317:ILE:CD1	2.40	0.51
1:P:446:ASP:OD1	1:P:472:ARG:HD3	2.11	0.51
1:G:232:ASN:O	1:G:232:ASN:ND2	2.44	0.50
1:M:246:LYS:NZ	1:M:302:VAL:HG13	2.26	0.50
1:M:722:TRP:CD1	2:N:264:PRO:HD3	2.46	0.50
3:O:10:ASN:N	3:O:10:ASN:OD1	2.43	0.50
1:P:363:ILE:HG23	1:P:374:VAL:HG13	1.93	0.50
3:R:161:ASN:O	3:R:164:LYS:HB2	2.10	0.50
3:R:5:PRO:O	3:R:245:VAL:HA	2.11	0.50
2:B:344:THR:HG22	2:B:436:LEU:HD13	1.93	0.50
2:B:495:LYS:HE2	2:B:499:LYS:HZ1	1.76	0.50
3:C:242:ILE:HG23	3:C:244:GLY:H	1.77	0.50
1:D:394:VAL:HG22	1:D:434:ARG:HH11	1.77	0.50
1:G:408:ILE:HD12	1:G:464:LEU:HD13	1.92	0.50
1:J:770:ASP:OD2	2:K:141:LEU:HG	2.12	0.50
3:L:242:ILE:HG23	3:L:244:GLY:H	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:372:HIS:CD2	3:L:410:TYR:HB3	2.47	0.50
1:M:292:LEU:CD1	1:M:343:LEU:HG	2.41	0.50
3:O:30:ARG:NE	3:O:168:ILE:HD12	2.25	0.50
3:R:158:THR:OG1	3:R:159:TYR:N	2.45	0.50
3:R:273:TRP:O	3:R:277:ILE:HG22	2.11	0.50
1:A:577:LEU:O	2:B:506:LYS:NZ	2.35	0.50
3:C:30:ARG:NE	3:C:168:ILE:HD12	2.25	0.50
1:D:363:ILE:HG22	1:D:374:VAL:HG22	1.93	0.50
3:F:161:ASN:O	3:F:164:LYS:HB2	2.10	0.50
3:F:273:TRP:O	3:F:277:ILE:HG22	2.11	0.50
3:I:209:ARG:HD3	3:I:209:ARG:H	1.77	0.50
2:K:367:PHE:CE2	3:L:222:LEU:HD21	2.46	0.50
1:M:420:GLU:HA	1:M:442:LEU:HD22	1.93	0.50
3:O:360:GLU:O	3:O:362:ALA:N	2.44	0.50
1:P:607:VAL:HB	1:P:731:LEU:HD13	1.94	0.50
2:Q:221:PRO:HA	2:Q:225:GLN:HB2	1.94	0.50
1:A:770:ASP:OD2	2:B:141:LEU:HG	2.12	0.50
1:D:246:LYS:NZ	1:D:302:VAL:HG13	2.27	0.50
3:F:360:GLU:O	3:F:362:ALA:N	2.44	0.50
2:H:359:ASP:N	2:H:359:ASP:OD2	2.44	0.50
3:I:273:TRP:O	3:I:277:ILE:HG22	2.11	0.50
1:J:217:ALA:HB2	1:J:233:VAL:HA	1.92	0.50
1:J:712:ASP:N	1:J:712:ASP:OD1	2.44	0.50
1:P:770:ASP:OD2	2:Q:141:LEU:HG	2.11	0.50
2:Q:344:THR:HG22	2:Q:436:LEU:HD13	1.92	0.50
3:R:209:ARG:H	3:R:209:ARG:HD3	1.76	0.50
3:R:26:TYR:CB	3:R:169:PRO:HB3	2.41	0.50
1:A:355:GLU:HB3	3:C:24:ILE:HG23	1.94	0.50
3:C:75:GLN:HA	3:C:78:ARG:NE	2.25	0.50
1:D:454:GLN:HE22	1:D:536:ASP:H	1.60	0.50
1:D:770:ASP:OD2	2:E:141:LEU:HG	2.11	0.50
2:E:163:SER:HA	2:E:230:ILE:HG22	1.94	0.50
3:F:242:ILE:HG23	3:F:244:GLY:H	1.76	0.50
3:I:201:SER:O	3:I:205:VAL:HG23	2.11	0.50
1:J:292:LEU:CD1	1:J:343:LEU:HG	2.41	0.50
1:J:292:LEU:HD11	1:J:343:LEU:HG	1.92	0.50
1:J:607:VAL:HB	1:J:731:LEU:HD13	1.94	0.50
1:J:667:ASP:OD1	1:J:667:ASP:N	2.44	0.50
3:L:360:GLU:O	3:L:362:ALA:N	2.45	0.50
3:L:5:PRO:O	3:L:245:VAL:HA	2.12	0.50
1:M:474:LYS:H	1:M:474:LYS:CD	2.24	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:161:ASN:O	3:O:164:LYS:HB2	2.11	0.50
1:P:722:TRP:CD1	2:Q:264:PRO:HD3	2.47	0.50
3:R:177:LEU:HD22	3:R:185:LYS:HG2	1.92	0.50
1:A:767:PRO:O	1:A:771:ILE:HG12	2.12	0.50
1:D:217:ALA:HB2	1:D:233:VAL:HA	1.93	0.50
1:D:446:ASP:OD1	1:D:472:ARG:HD3	2.12	0.50
1:D:603:ARG:O	1:D:607:VAL:HG23	2.12	0.50
1:G:420:GLU:HA	1:G:442:LEU:HD22	1.93	0.50
1:G:722:TRP:CD1	2:H:264:PRO:HD3	2.46	0.50
2:H:344:THR:HG22	2:H:436:LEU:HD13	1.94	0.50
1:J:317:ILE:HG13	1:J:326:ILE:HD13	1.93	0.50
1:J:770:ASP:HB2	2:K:145:ASN:OD1	2.12	0.50
1:M:599:LYS:HG2	2:N:272:GLN:OE1	2.12	0.50
2:N:344:THR:HG22	2:N:436:LEU:HD13	1.92	0.50
3:O:177:LEU:HD22	3:O:185:LYS:HG2	1.93	0.50
3:O:26:TYR:CB	3:O:169:PRO:HB3	2.41	0.50
1:P:217:ALA:HB2	1:P:233:VAL:HA	1.93	0.50
2:Q:321:ASP:O	2:Q:324:ARG:N	2.24	0.50
2:Q:409:ALA:O	2:Q:413:LEU:CB	2.53	0.50
1:A:454:GLN:HE22	1:A:536:ASP:H	1.60	0.50
3:F:213:ILE:HG12	3:F:242:ILE:HD13	1.93	0.50
1:G:446:ASP:OD1	1:G:472:ARG:HD3	2.11	0.50
1:J:246:LYS:NZ	1:J:302:VAL:HG13	2.27	0.50
2:K:221:PRO:HA	2:K:225:GLN:HB2	1.94	0.50
3:L:273:TRP:O	3:L:277:ILE:HG22	2.10	0.50
1:M:232:ASN:O	1:M:232:ASN:ND2	2.44	0.50
1:P:355:GLU:HB3	3:R:24:ILE:HG23	1.93	0.50
3:C:372:HIS:CD2	3:C:410:TYR:HB3	2.47	0.50
3:F:372:HIS:CD2	3:F:410:TYR:HB3	2.47	0.50
3:I:177:LEU:HD22	3:I:185:LYS:HG2	1.93	0.50
1:J:767:PRO:O	1:J:771:ILE:HG12	2.12	0.50
2:K:409:ALA:O	2:K:413:LEU:CB	2.52	0.50
3:L:161:ASN:O	3:L:164:LYS:HB2	2.11	0.50
1:M:394:VAL:HG22	1:M:434:ARG:HH11	1.77	0.50
2:N:193:PHE:HD1	2:N:219:ILE:HD11	1.76	0.50
1:P:712:ASP:N	1:P:712:ASP:OD1	2.44	0.50
3:R:213:ILE:HG12	3:R:242:ILE:HD13	1.93	0.50
3:R:242:ILE:HG23	3:R:244:GLY:H	1.77	0.50
3:R:360:GLU:O	3:R:362:ALA:N	2.44	0.50
1:A:365:TRP:HE3	1:A:372:ILE:HG22	1.77	0.50
1:A:408:ILE:HG12	1:A:408:ILE:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:425:GLY:HA2	1:A:435:ARG:HB2	1.93	0.50
1:A:751:SER:O	1:A:753:PHE:N	2.45	0.50
3:C:209:ARG:H	3:C:209:ARG:HD3	1.77	0.50
1:D:265:THR:OG1	1:D:268:SER:N	2.42	0.50
1:D:712:ASP:OD1	1:D:712:ASP:N	2.43	0.50
3:F:177:LEU:HD22	3:F:185:LYS:HG2	1.93	0.50
3:F:209:ARG:HD3	3:F:209:ARG:H	1.76	0.50
1:J:355:GLU:HB3	3:L:24:ILE:HG23	1.93	0.50
2:K:252:LEU:HD22	2:K:306:VAL:HG11	1.93	0.50
1:A:317:ILE:HG13	1:A:326:ILE:HD13	1.93	0.49
2:B:163:SER:HA	2:B:230:ILE:HG22	1.94	0.49
3:C:360:GLU:O	3:C:362:ALA:N	2.44	0.49
1:D:408:ILE:HB	1:D:453:VAL:HG21	1.94	0.49
1:G:246:LYS:HD2	1:G:303:VAL:HG13	1.94	0.49
2:H:163:SER:HA	2:H:230:ILE:HG22	1.94	0.49
1:G:599:LYS:HG2	2:H:272:GLN:OE1	2.12	0.49
1:M:712:ASP:N	1:M:712:ASP:OD1	2.44	0.49
3:O:5:PRO:O	3:O:245:VAL:HA	2.11	0.49
1:P:265:THR:OG1	1:P:268:SER:N	2.41	0.49
1:P:365:TRP:HE3	1:P:372:ILE:HG22	1.77	0.49
1:D:317:ILE:HG13	1:D:326:ILE:HD13	1.94	0.49
1:G:473:HIS:ND1	1:G:473:HIS:O	2.43	0.49
2:H:502:ILE:O	2:H:506:LYS:HB2	2.12	0.49
3:O:213:ILE:HG12	3:O:242:ILE:HD13	1.93	0.49
3:O:372:HIS:CD2	3:O:410:TYR:HB3	2.47	0.49
1:P:394:VAL:HG22	1:P:434:ARG:HH11	1.77	0.49
3:C:201:SER:O	3:C:205:VAL:HG23	2.12	0.49
1:D:474:LYS:H	1:D:474:LYS:CD	2.25	0.49
2:E:252:LEU:HD22	2:E:306:VAL:HG11	1.94	0.49
1:G:394:VAL:HG22	1:G:434:ARG:HH11	1.77	0.49
3:I:242:ILE:HG23	3:I:244:GLY:H	1.77	0.49
1:J:474:LYS:CD	1:J:474:LYS:H	2.25	0.49
2:K:163:SER:HA	2:K:230:ILE:HG22	1.94	0.49
1:P:767:PRO:O	1:P:771:ILE:HG12	2.12	0.49
1:A:722:TRP:CD1	2:B:264:PRO:HD3	2.47	0.49
2:B:274:ILE:HG23	2:B:282:ARG:NH2	2.27	0.49
2:E:193:PHE:HD1	2:E:219:ILE:HD11	1.76	0.49
1:G:246:LYS:NZ	1:G:302:VAL:HG13	2.27	0.49
2:H:414:TYR:CE2	2:H:419:LEU:HB3	2.48	0.49
3:I:360:GLU:O	3:I:362:ALA:N	2.45	0.49
1:J:394:VAL:HG22	1:J:434:ARG:HH11	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:446:ASP:OD1	1:J:472:ARG:HD3	2.13	0.49
3:L:436:LYS:HA	3:L:439:GLU:HB2	1.94	0.49
1:M:363:ILE:HG23	1:M:374:VAL:HG13	1.95	0.49
1:M:378:SER:HB2	1:M:379:LYS:HD2	1.94	0.49
2:Q:359:ASP:N	2:Q:359:ASP:OD2	2.45	0.49
2:Q:414:TYR:CE2	2:Q:419:LEU:HB3	2.48	0.49
3:R:10:ASN:N	3:R:10:ASN:OD1	2.43	0.49
1:A:408:ILE:HB	1:A:453:VAL:HG21	1.93	0.49
1:D:420:GLU:HA	1:D:442:LEU:HD22	1.93	0.49
1:D:767:PRO:O	1:D:771:ILE:HG12	2.12	0.49
3:I:158:THR:OG1	3:I:159:TYR:N	2.46	0.49
1:J:363:ILE:HG23	1:J:374:VAL:HG13	1.93	0.49
2:K:498:LEU:O	2:K:502:ILE:HG23	2.12	0.49
1:M:603:ARG:O	1:M:607:VAL:HG23	2.13	0.49
1:M:751:SER:O	1:M:753:PHE:N	2.46	0.49
3:R:372:HIS:CD2	3:R:410:TYR:HB3	2.47	0.49
1:A:277:VAL:HG12	1:A:284:VAL:HA	1.95	0.49
1:D:365:TRP:HE3	1:D:372:ILE:HG22	1.77	0.49
1:G:426:ALA:C	1:G:433:VAL:HG11	2.33	0.49
1:G:736:ILE:HD11	2:H:254:LEU:HD13	1.94	0.49
2:H:274:ILE:HG23	2:H:282:ARG:NH2	2.27	0.49
2:K:502:ILE:O	2:K:506:LYS:HB2	2.13	0.49
1:M:355:GLU:HB3	3:O:24:ILE:HG23	1.94	0.49
1:M:770:ASP:HB2	2:N:145:ASN:OD1	2.12	0.49
1:A:246:LYS:NZ	1:A:302:VAL:HG13	2.28	0.49
1:G:355:GLU:HB3	3:I:24:ILE:HG23	1.95	0.49
1:G:363:ILE:HG22	1:G:374:VAL:HG22	1.94	0.49
2:K:274:ILE:HG23	2:K:282:ARG:NH2	2.28	0.49
1:P:246:LYS:HD2	1:P:303:VAL:HG13	1.94	0.49
3:R:436:LYS:HA	3:R:439:GLU:HB2	1.94	0.49
1:A:394:VAL:HG22	1:A:434:ARG:HH11	1.78	0.49
1:D:246:LYS:HD2	1:D:303:VAL:HG13	1.95	0.49
1:D:577:LEU:O	2:E:506:LYS:NZ	2.35	0.49
3:F:201:SER:O	3:F:205:VAL:HG23	2.12	0.49
1:G:650:LEU:HD22	2:H:242:PHE:HA	1.95	0.49
2:H:409:ALA:O	2:H:413:LEU:CB	2.52	0.49
2:K:359:ASP:N	2:K:359:ASP:OD2	2.46	0.49
3:L:201:SER:O	3:L:205:VAL:HG23	2.13	0.49
1:M:667:ASP:N	1:M:667:ASP:OD1	2.44	0.49
1:P:317:ILE:HG13	1:P:326:ILE:HD13	1.95	0.49
2:Q:502:ILE:O	2:Q:506:LYS:HB2	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:363:ILE:HG22	1:A:374:VAL:HG22	1.93	0.49
1:A:603:ARG:O	1:A:607:VAL:HG23	2.13	0.49
1:A:762:ARG:HG3	2:B:139:LYS:HE3	1.95	0.49
2:B:193:PHE:HD1	2:B:219:ILE:HD11	1.77	0.49
1:D:378:SER:HB2	1:D:379:LYS:HD2	1.95	0.49
2:H:367:PHE:CE2	3:I:222:LEU:HD21	2.48	0.49
3:I:372:HIS:CD2	3:I:410:TYR:HB3	2.48	0.49
1:J:408:ILE:O	1:J:408:ILE:HG12	2.10	0.49
2:K:119:LEU:HD13	2:K:125:PHE:CG	2.48	0.49
1:M:365:TRP:HE3	1:M:372:ILE:HG22	1.77	0.49
1:M:767:PRO:O	1:M:771:ILE:HG12	2.13	0.49
1:P:603:ARG:O	1:P:607:VAL:HG23	2.12	0.49
1:A:474:LYS:H	1:A:474:LYS:CD	2.25	0.49
2:B:414:TYR:CE2	2:B:419:LEU:HB3	2.48	0.49
1:A:355:GLU:HA	3:C:24:ILE:HD12	1.95	0.49
1:D:607:VAL:HB	1:D:731:LEU:HD13	1.94	0.49
2:E:321:ASP:O	2:E:324:ARG:N	2.24	0.49
3:F:222:LEU:HD23	3:F:226:ARG:NH2	2.28	0.49
3:I:436:LYS:HA	3:I:439:GLU:HB2	1.95	0.49
1:J:420:GLU:HA	1:J:442:LEU:HD22	1.93	0.49
2:N:119:LEU:HD13	2:N:125:PHE:CG	2.48	0.49
1:M:736:ILE:HD11	2:N:254:LEU:HD13	1.95	0.49
2:N:498:LEU:O	2:N:502:ILE:HG23	2.13	0.49
3:O:201:SER:O	3:O:205:VAL:HG23	2.12	0.49
1:P:246:LYS:NZ	1:P:302:VAL:HG13	2.28	0.49
1:P:363:ILE:HG22	1:P:374:VAL:HG22	1.94	0.49
1:P:770:ASP:HB2	2:Q:145:ASN:OD1	2.13	0.49
2:Q:119:LEU:HD13	2:Q:125:PHE:CG	2.48	0.49
3:R:75:GLN:HA	3:R:78:ARG:NE	2.25	0.49
1:G:365:TRP:HE3	1:G:372:ILE:HG22	1.78	0.48
2:H:193:PHE:HD1	2:H:219:ILE:HD11	1.77	0.48
3:I:222:LEU:HD23	3:I:226:ARG:NH2	2.28	0.48
2:K:193:PHE:HD1	2:K:219:ILE:HD11	1.77	0.48
1:M:650:LEU:HD22	2:N:242:PHE:HA	1.95	0.48
1:M:656:HIS:CE1	2:N:171:HIS:CE1	3.00	0.48
2:N:137:TRP:CE3	2:N:140:ILE:HD11	2.48	0.48
2:N:414:TYR:CE2	2:N:419:LEU:HB3	2.48	0.48
2:N:502:ILE:O	2:N:506:LYS:HB2	2.13	0.48
1:P:426:ALA:C	1:P:433:VAL:HG11	2.33	0.48
1:P:736:ILE:HD11	2:Q:254:LEU:HD13	1.95	0.48
1:A:321:LYS:N	1:A:321:LYS:HD3	2.21	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:363:ILE:HG23	1:A:374:VAL:HG13	1.94	0.48
1:D:770:ASP:HB2	2:E:145:ASN:OD1	2.13	0.48
2:E:502:ILE:O	2:E:506:LYS:HB2	2.13	0.48
1:G:656:HIS:CE1	2:H:171:HIS:CE1	3.01	0.48
2:H:287:TRP:CE2	2:H:289:ARG:HB3	2.48	0.48
1:J:365:TRP:HE3	1:J:372:ILE:HG22	1.77	0.48
1:J:426:ALA:C	1:J:433:VAL:HG11	2.34	0.48
1:M:363:ILE:HG22	1:M:374:VAL:HG22	1.93	0.48
3:R:201:SER:O	3:R:205:VAL:HG23	2.12	0.48
2:B:252:LEU:HD22	2:B:306:VAL:HG11	1.94	0.48
2:E:287:TRP:CE2	2:E:289:ARG:HB3	2.49	0.48
2:E:498:LEU:O	2:E:502:ILE:HG23	2.14	0.48
1:G:454:GLN:HE22	1:G:536:ASP:H	1.61	0.48
1:G:473:HIS:HD2	1:G:475:ARG:HH11	1.62	0.48
2:H:119:LEU:HD13	2:H:125:PHE:CG	2.49	0.48
2:Q:287:TRP:CE2	2:Q:289:ARG:HB3	2.49	0.48
2:Q:367:PHE:CE2	3:R:222:LEU:HD21	2.48	0.48
1:A:426:ALA:C	1:A:433:VAL:HG11	2.34	0.48
1:A:607:VAL:HB	1:A:731:LEU:HD13	1.94	0.48
3:C:158:THR:OG1	3:C:159:TYR:N	2.46	0.48
2:B:367:PHE:CE2	3:C:222:LEU:HD21	2.49	0.48
1:D:425:GLY:HA2	1:D:435:ARG:HB2	1.95	0.48
3:F:436:LYS:HA	3:F:439:GLU:HB2	1.94	0.48
1:G:277:VAL:HG12	1:G:284:VAL:HA	1.95	0.48
1:G:474:LYS:CD	1:G:474:LYS:H	2.26	0.48
1:G:770:ASP:HB2	2:H:145:ASN:OD1	2.14	0.48
1:J:363:ILE:HG22	1:J:374:VAL:HG22	1.95	0.48
2:K:414:TYR:CE2	2:K:419:LEU:HB3	2.48	0.48
3:L:222:LEU:HD23	3:L:226:ARG:NH2	2.27	0.48
1:P:751:SER:O	1:P:753:PHE:N	2.46	0.48
2:Q:274:ILE:HG23	2:Q:282:ARG:NH2	2.28	0.48
1:D:426:ALA:C	1:D:433:VAL:HG11	2.33	0.48
3:F:158:THR:OG1	3:F:159:TYR:N	2.47	0.48
1:G:378:SER:HB2	1:G:379:LYS:HD2	1.95	0.48
1:J:265:THR:OG1	1:J:268:SER:N	2.41	0.48
1:J:321:LYS:HD3	1:J:321:LYS:N	2.21	0.48
1:J:365:TRP:CB	1:J:372:ILE:HA	2.44	0.48
2:N:221:PRO:HA	2:N:225:GLN:HB2	1.94	0.48
2:N:359:ASP:OD2	2:N:359:ASP:N	2.46	0.48
3:O:222:LEU:HD23	3:O:226:ARG:NH2	2.28	0.48
1:P:425:GLY:HA2	1:P:435:ARG:HB2	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:161:THR:OG1	2:B:162:ILE:N	2.47	0.48
2:E:414:TYR:CE2	2:E:419:LEU:HB3	2.47	0.48
1:G:363:ILE:HG23	1:G:374:VAL:HG13	1.94	0.48
1:G:408:ILE:O	1:G:408:ILE:HG12	2.10	0.48
2:H:221:PRO:HA	2:H:225:GLN:HB2	1.94	0.48
1:J:355:GLU:HA	3:L:24:ILE:HD12	1.96	0.48
3:O:158:THR:OG1	3:O:159:TYR:N	2.47	0.48
2:Q:252:LEU:HD22	2:Q:306:VAL:HG11	1.94	0.48
1:D:751:SER:O	1:D:753:PHE:N	2.46	0.48
1:G:751:SER:O	1:G:753:PHE:N	2.46	0.48
2:H:137:TRP:CH2	2:H:141:LEU:HD13	2.49	0.48
1:J:246:LYS:HD2	1:J:303:VAL:HG13	1.96	0.48
1:M:277:VAL:HG12	1:M:284:VAL:HA	1.96	0.48
3:O:209:ARG:H	3:O:209:ARG:HD3	1.77	0.48
1:P:577:LEU:O	2:Q:506:LYS:NZ	2.38	0.48
2:Q:161:THR:OG1	2:Q:162:ILE:N	2.47	0.48
1:P:656:HIS:CE1	2:Q:171:HIS:CE1	3.02	0.48
3:F:11:ARG:H	3:F:11:ARG:HG3	1.49	0.48
1:G:317:ILE:HG13	1:G:326:ILE:HD13	1.95	0.48
1:M:762:ARG:HG3	2:N:139:LYS:HE3	1.96	0.48
1:P:454:GLN:HE22	1:P:536:ASP:H	1.62	0.48
3:C:141:TRP:H	3:C:141:TRP:HD1	1.58	0.48
1:D:473:HIS:HD2	1:D:475:ARG:HH11	1.61	0.48
1:D:762:ARG:HG3	2:E:139:LYS:HE3	1.96	0.48
2:E:119:LEU:HD13	2:E:125:PHE:CG	2.49	0.48
2:E:137:TRP:CE3	2:E:140:ILE:HD11	2.49	0.48
1:G:662:LEU:HD13	1:G:665:ASN:CG	2.34	0.48
1:J:473:HIS:HD2	1:J:475:ARG:HH11	1.62	0.48
1:J:736:ILE:HD11	2:K:254:LEU:HD13	1.96	0.48
3:L:246:GLN:HG2	3:L:247:ILE:H	1.79	0.48
3:L:250:LEU:HD12	3:L:274:MET:HE1	1.96	0.48
2:N:287:TRP:CE2	2:N:289:ARG:HB3	2.48	0.48
2:Q:163:SER:HA	2:Q:230:ILE:HG22	1.95	0.48
2:Q:498:LEU:O	2:Q:502:ILE:HG23	2.14	0.48
1:P:573:GLU:HB3	2:Q:499:LYS:HD3	1.96	0.48
2:B:502:ILE:O	2:B:506:LYS:HB2	2.14	0.48
2:E:194:GLN:OE1	2:E:194:GLN:N	2.47	0.48
1:G:321:LYS:N	1:G:321:LYS:HD3	2.22	0.48
1:G:425:GLY:HA2	1:G:435:ARG:HB2	1.96	0.48
3:O:436:LYS:HA	3:O:439:GLU:HB2	1.94	0.48
2:B:109:GLN:OE1	2:B:137:TRP:NE1	2.42	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:287:TRP:CE2	2:B:289:ARG:HB3	2.48	0.47
2:B:498:LEU:O	2:B:502:ILE:HG23	2.13	0.47
3:C:76:LYS:HA	3:C:79:ARG:HB2	1.96	0.47
1:G:762:ARG:HG3	2:H:139:LYS:HE3	1.96	0.47
1:J:277:VAL:HG12	1:J:284:VAL:HA	1.95	0.47
1:M:473:HIS:HD2	1:M:475:ARG:HH11	1.62	0.47
1:P:378:SER:HB2	1:P:379:LYS:HD2	1.95	0.47
1:P:667:ASP:N	1:P:667:ASP:OD1	2.44	0.47
2:Q:137:TRP:CE3	2:Q:140:ILE:HD11	2.49	0.47
3:R:222:LEU:HD23	3:R:226:ARG:NH2	2.29	0.47
3:R:347:ASP:O	3:R:351:GLU:CB	2.61	0.47
1:A:426:ALA:O	1:A:433:VAL:HG11	2.14	0.47
3:C:436:LYS:HA	3:C:439:GLU:HB2	1.94	0.47
3:I:246:GLN:HG2	3:I:247:ILE:H	1.79	0.47
1:J:762:ARG:HG3	2:K:139:LYS:HE3	1.96	0.47
2:K:161:THR:OG1	2:K:162:ILE:N	2.48	0.47
2:K:287:TRP:CE2	2:K:289:ARG:HB3	2.48	0.47
2:K:502:ILE:HA	2:K:505:ILE:HG22	1.95	0.47
1:M:355:GLU:HA	3:O:24:ILE:HD12	1.96	0.47
1:M:426:ALA:C	1:M:433:VAL:HG11	2.34	0.47
1:M:626:LEU:HD11	1:M:665:ASN:HB2	1.96	0.47
2:B:119:LEU:HD13	2:B:125:PHE:CG	2.49	0.47
2:B:502:ILE:HA	2:B:505:ILE:HG22	1.96	0.47
1:D:355:GLU:HA	3:F:24:ILE:HD12	1.96	0.47
2:E:502:ILE:HA	2:E:505:ILE:HG22	1.95	0.47
3:F:246:GLN:HG2	3:F:247:ILE:H	1.79	0.47
3:F:75:GLN:HA	3:F:78:ARG:NE	2.25	0.47
2:K:484:ALA:O	2:K:488:LEU:HG	2.13	0.47
2:N:161:THR:OG1	2:N:162:ILE:N	2.47	0.47
2:N:250:GLN:HB3	2:N:267:TYR:OH	2.14	0.47
2:N:252:LEU:HD22	2:N:306:VAL:HG11	1.95	0.47
3:O:16:ARG:NH2	3:O:183:GLU:OE2	2.48	0.47
3:O:295:PRO:HB3	3:O:296:PRO:HD2	1.96	0.47
1:P:377:ARG:HG3	1:P:377:ARG:H	1.56	0.47
1:A:473:HIS:HD2	1:A:475:ARG:HH11	1.63	0.47
1:D:277:VAL:HG12	1:D:284:VAL:HA	1.95	0.47
1:D:321:LYS:HD3	1:D:321:LYS:N	2.20	0.47
1:D:736:ILE:HD11	2:E:254:LEU:HD13	1.96	0.47
1:G:619:GLU:OE2	1:G:670:ALA:N	2.47	0.47
3:L:141:TRP:HD1	3:L:141:TRP:H	1.58	0.47
3:L:158:THR:OG1	3:L:159:TYR:N	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:662:LEU:HD13	1:M:665:ASN:CG	2.35	0.47
2:N:163:SER:HA	2:N:230:ILE:HG22	1.95	0.47
1:P:762:ARG:HG3	2:Q:139:LYS:HE3	1.97	0.47
3:R:76:LYS:HA	3:R:79:ARG:HB2	1.95	0.47
1:A:362:ARG:HB3	1:A:375:PHE:HB2	1.97	0.47
2:B:194:GLN:OE1	2:B:194:GLN:N	2.48	0.47
1:D:365:TRP:CB	1:D:372:ILE:HA	2.44	0.47
2:E:178:THR:HG21	2:E:227:TYR:OH	2.15	0.47
1:G:365:TRP:CB	1:G:372:ILE:HA	2.44	0.47
1:G:426:ALA:O	1:G:433:VAL:HG11	2.14	0.47
2:H:137:TRP:CE3	2:H:140:ILE:HD11	2.49	0.47
2:H:161:THR:OG1	2:H:162:ILE:N	2.48	0.47
2:H:498:LEU:O	2:H:502:ILE:HG23	2.15	0.47
1:J:656:HIS:CE1	2:K:171:HIS:CE1	3.03	0.47
1:J:751:SER:O	1:J:753:PHE:N	2.46	0.47
2:K:239:PHE:HB2	2:K:245:SER:OG	2.15	0.47
3:L:76:LYS:HA	3:L:79:ARG:HB2	1.96	0.47
3:O:308:PHE:HD1	3:O:309:ALA:N	2.13	0.47
1:P:426:ALA:O	1:P:433:VAL:HG11	2.14	0.47
2:Q:194:GLN:OE1	2:Q:194:GLN:N	2.47	0.47
2:Q:484:ALA:O	2:Q:488:LEU:HG	2.14	0.47
1:A:378:SER:HB2	1:A:379:LYS:HD2	1.95	0.47
3:C:16:ARG:NH2	3:C:183:GLU:OE2	2.48	0.47
3:C:246:GLN:HG2	3:C:247:ILE:H	1.80	0.47
3:F:76:LYS:HA	3:F:79:ARG:HB2	1.96	0.47
3:I:75:GLN:HA	3:I:78:ARG:NE	2.25	0.47
2:K:495:LYS:CG	2:K:499:LYS:HZ1	2.28	0.47
1:M:619:GLU:OE2	1:M:670:ALA:N	2.48	0.47
1:M:778:ASP:CG	1:M:779:ASP:H	2.18	0.47
3:C:302:ARG:HG2	3:C:302:ARG:H	1.45	0.47
1:D:656:HIS:CE1	2:E:171:HIS:CE1	3.03	0.47
2:K:137:TRP:CE3	2:K:140:ILE:HD11	2.49	0.47
3:L:75:GLN:HA	3:L:78:ARG:NE	2.25	0.47
3:C:171:ARG:HH22	2:N:444:GLU:HG2	1.79	0.47
1:A:778:ASP:CG	1:A:779:ASP:H	2.18	0.47
3:C:295:PRO:HB3	3:C:296:PRO:HD2	1.97	0.47
2:H:194:GLN:N	2:H:194:GLN:OE1	2.47	0.47
2:H:414:TYR:HE2	2:H:419:LEU:HB3	1.79	0.47
1:J:662:LEU:HD13	1:J:665:ASN:CG	2.35	0.47
1:M:321:LYS:N	1:M:321:LYS:HD3	2.23	0.47
2:N:414:TYR:HE2	2:N:419:LEU:HB3	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:573:GLU:HB3	2:N:499:LYS:HD3	1.96	0.47
2:N:367:PHE:CE2	3:O:222:LEU:HD21	2.49	0.47
1:P:381:ILE:HA	1:P:391:THR:O	2.15	0.47
1:P:778:ASP:CG	1:P:779:ASP:H	2.18	0.47
1:A:365:TRP:CB	1:A:372:ILE:HA	2.44	0.47
2:B:494:SER:HB2	2:B:497:GLN:H	1.80	0.47
1:D:363:ILE:HG23	1:D:374:VAL:HG13	1.95	0.47
2:E:161:THR:OG1	2:E:162:ILE:N	2.48	0.47
1:D:650:LEU:HD22	2:E:242:PHE:HA	1.97	0.47
1:G:626:LEU:HA	1:G:626:LEU:HD22	1.65	0.47
2:H:502:ILE:HA	2:H:505:ILE:HG22	1.96	0.47
2:H:512:ARG:HA	2:H:512:ARG:HD3	1.83	0.47
3:I:250:LEU:HD12	3:I:274:MET:HE1	1.96	0.47
3:I:308:PHE:HD1	3:I:309:ALA:N	2.13	0.47
1:J:378:SER:HB2	1:J:379:LYS:HD2	1.95	0.47
3:L:417:ILE:O	3:L:420:ASP:HB3	2.14	0.47
1:M:577:LEU:O	2:N:506:LYS:NZ	2.42	0.47
2:N:502:ILE:HA	2:N:505:ILE:HG22	1.97	0.47
1:P:753:PHE:HA	1:P:753:PHE:HD1	1.65	0.47
1:P:599:LYS:HG2	2:Q:272:GLN:OE1	2.15	0.47
1:D:381:ILE:HA	1:D:391:THR:O	2.15	0.47
1:M:246:LYS:HD2	1:M:303:VAL:HG13	1.97	0.47
3:O:246:GLN:HG2	3:O:247:ILE:H	1.79	0.47
1:P:277:VAL:HG12	1:P:284:VAL:HA	1.95	0.47
1:P:365:TRP:CB	1:P:372:ILE:HA	2.45	0.47
1:P:421:ILE:CG2	1:P:423:ILE:HG13	2.45	0.47
3:O:171:ARG:HH22	2:Q:444:GLU:HG2	1.79	0.47
1:A:656:HIS:CE1	2:B:171:HIS:CE1	3.02	0.47
1:A:757:GLN:HE21	1:A:758:ASN:N	2.13	0.47
2:B:137:TRP:CE3	2:B:140:ILE:HD11	2.50	0.47
3:C:402:ASN:O	3:C:406:LYS:HG2	2.15	0.47
1:D:427:SER:HB2	1:D:429:SER:O	2.15	0.47
1:D:757:GLN:HE21	1:D:758:ASN:N	2.13	0.47
2:E:250:GLN:HB3	2:E:267:TYR:OH	2.14	0.47
1:G:577:LEU:O	2:H:506:LYS:NZ	2.42	0.47
2:K:178:THR:HG22	2:K:303:GLU:OE1	2.15	0.47
3:L:295:PRO:HB3	3:L:296:PRO:HD2	1.96	0.47
2:N:274:ILE:HG23	2:N:282:ARG:NH2	2.30	0.47
3:R:150:GLN:H	3:R:150:GLN:HG2	1.35	0.47
2:B:414:TYR:HE2	2:B:419:LEU:HB3	1.80	0.46
3:C:250:LEU:HD12	3:C:274:MET:HE1	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:417:ILE:O	3:C:420:ASP:HB3	2.16	0.46
2:E:137:TRP:CH2	2:E:141:LEU:HD13	2.50	0.46
2:E:359:ASP:N	2:E:359:ASP:OD2	2.46	0.46
2:H:484:ALA:O	2:H:488:LEU:HG	2.14	0.46
3:I:9:THR:O	3:I:13:PHE:HD2	1.98	0.46
1:J:778:ASP:CG	1:J:779:ASP:H	2.18	0.46
3:L:231:LEU:O	3:L:235:ILE:HG12	2.15	0.46
1:M:365:TRP:CB	1:M:372:ILE:HA	2.44	0.46
2:N:194:GLN:OE1	2:N:194:GLN:N	2.48	0.46
3:O:417:ILE:O	3:O:420:ASP:HB3	2.15	0.46
1:P:626:LEU:HD11	1:P:665:ASN:HB2	1.97	0.46
1:P:662:LEU:HD13	1:P:665:ASN:CG	2.36	0.46
2:Q:178:THR:HG22	2:Q:303:GLU:OE1	2.14	0.46
2:Q:414:TYR:HE2	2:Q:419:LEU:HB3	1.80	0.46
3:R:246:GLN:HG2	3:R:247:ILE:H	1.79	0.46
1:A:183:ASP:HB3	1:A:247:ILE:HG22	1.98	0.46
2:B:108:PHE:CD1	2:B:156:LEU:HB3	2.51	0.46
2:B:359:ASP:OD2	2:B:359:ASP:N	2.47	0.46
3:C:308:PHE:HD1	3:C:309:ALA:N	2.13	0.46
1:D:753:PHE:HD1	1:D:753:PHE:HA	1.65	0.46
2:H:435:GLN:H	2:H:435:GLN:HG3	1.42	0.46
3:I:76:LYS:HA	3:I:79:ARG:HB2	1.96	0.46
1:J:619:GLU:OE2	1:J:670:ALA:N	2.48	0.46
2:K:178:THR:HG21	2:K:227:TYR:OH	2.15	0.46
1:M:425:GLY:HA2	1:M:435:ARG:HB2	1.97	0.46
1:P:660:LYS:HD3	1:P:660:LYS:HA	1.66	0.46
1:P:746:ARG:HG2	1:P:747:LEU:N	2.31	0.46
2:Q:137:TRP:CH2	2:Q:141:LEU:HD13	2.51	0.46
2:Q:386:LEU:HD13	3:R:241:ARG:NH2	2.30	0.46
1:D:426:ALA:O	1:D:433:VAL:HG11	2.14	0.46
1:D:60:VAL:O	1:D:61:VAL:HG23	2.15	0.46
1:G:355:GLU:HA	3:I:24:ILE:HD12	1.98	0.46
1:J:757:GLN:HE21	1:J:758:ASN:N	2.13	0.46
3:L:347:ASP:O	3:L:351:GLU:CB	2.61	0.46
1:M:426:ALA:O	1:M:433:VAL:HG11	2.14	0.46
1:M:740:ILE:O	1:M:744:LEU:HG	2.15	0.46
2:N:494:SER:HB2	2:N:497:GLN:H	1.81	0.46
3:O:76:LYS:HA	3:O:79:ARG:HB2	1.96	0.46
1:P:473:HIS:HD2	1:P:475:ARG:HH11	1.63	0.46
3:R:402:ASN:O	3:R:406:LYS:HG2	2.16	0.46
2:B:137:TRP:CH2	2:B:141:LEU:HD13	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:447:ALA:HA	2:B:450:THR:HB	1.97	0.46
1:D:656:HIS:CD2	1:D:656:HIS:N	2.84	0.46
3:F:171:ARG:HH22	2:H:444:GLU:HG2	1.80	0.46
2:E:367:PHE:CE2	3:F:222:LEU:HD21	2.50	0.46
3:F:295:PRO:HB3	3:F:296:PRO:HD2	1.96	0.46
3:F:347:ASP:O	3:F:351:GLU:CB	2.62	0.46
1:G:183:ASP:HB3	1:G:247:ILE:HG22	1.98	0.46
1:G:427:SER:HB2	1:G:429:SER:O	2.16	0.46
2:H:250:GLN:HB3	2:H:267:TYR:OH	2.15	0.46
2:K:137:TRP:CH2	2:K:141:LEU:HD13	2.51	0.46
3:L:308:PHE:HD1	3:L:309:ALA:N	2.14	0.46
1:P:427:SER:HB2	1:P:429:SER:O	2.15	0.46
2:B:105:LEU:HD13	2:B:141:LEU:HD11	1.98	0.46
3:C:231:LEU:O	3:C:235:ILE:HG12	2.16	0.46
3:F:308:PHE:HD1	3:F:309:ALA:N	2.13	0.46
1:G:362:ARG:HB3	1:G:375:PHE:HB2	1.97	0.46
3:I:417:ILE:O	3:I:420:ASP:HB3	2.15	0.46
1:J:426:ALA:O	1:J:433:VAL:HG11	2.15	0.46
1:J:626:LEU:HD11	1:J:665:ASN:HB2	1.97	0.46
3:L:402:ASN:O	3:L:406:LYS:HG2	2.15	0.46
1:M:317:ILE:HG13	1:M:326:ILE:HD13	1.96	0.46
1:M:479:HIS:NE2	1:M:491:SER:OG	2.27	0.46
1:M:574:TRP:CH2	2:N:495:LYS:HD2	2.51	0.46
1:P:650:LEU:HD22	2:Q:242:PHE:HA	1.98	0.46
1:P:694:ILE:HD12	1:P:746:ARG:HG3	1.97	0.46
1:P:757:GLN:HE21	1:P:758:ASN:N	2.14	0.46
3:R:158:THR:HG23	3:R:161:ASN:H	1.81	0.46
1:A:746:ARG:HG2	1:A:747:LEU:N	2.30	0.46
1:D:662:LEU:HD13	1:D:665:ASN:CG	2.35	0.46
1:D:694:ILE:HD12	1:D:746:ARG:HG3	1.98	0.46
1:D:746:ARG:HG2	1:D:747:LEU:N	2.31	0.46
3:F:417:ILE:O	3:F:420:ASP:HB3	2.16	0.46
3:I:295:PRO:HB3	3:I:296:PRO:HD2	1.97	0.46
2:K:105:LEU:HD13	2:K:141:LEU:HD11	1.98	0.46
2:K:194:GLN:OE1	2:K:194:GLN:N	2.48	0.46
1:M:746:ARG:HG2	1:M:747:LEU:N	2.31	0.46
3:R:308:PHE:HD1	3:R:309:ALA:N	2.13	0.46
1:A:246:LYS:HD2	1:A:303:VAL:HG13	1.97	0.46
3:C:222:LEU:HD23	3:C:226:ARG:NH2	2.30	0.46
1:D:323:ASN:N	1:D:323:ASN:OD1	2.48	0.46
1:D:619:GLU:OE2	1:D:670:ALA:N	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:599:LYS:HG2	2:E:272:GLN:OE1	2.15	0.46
2:E:414:TYR:HE2	2:E:419:LEU:HB3	1.79	0.46
2:E:447:ALA:HA	2:E:450:THR:HB	1.98	0.46
1:J:245:ILE:HG23	1:J:263:ILE:HG22	1.98	0.46
2:K:137:TRP:O	2:K:141:LEU:HB2	2.16	0.46
2:K:250:GLN:HB3	2:K:267:TYR:OH	2.15	0.46
3:R:235:ILE:H	3:R:235:ILE:HG12	1.59	0.46
1:A:381:ILE:HA	1:A:391:THR:O	2.15	0.46
1:A:470:SER:O	1:A:504:THR:HG22	2.16	0.46
1:A:740:ILE:O	1:A:744:LEU:HG	2.15	0.46
2:B:136:ILE:HG12	2:B:243:PHE:CZ	2.51	0.46
3:C:158:THR:HG23	3:C:161:ASN:H	1.81	0.46
1:D:760:ILE:O	1:D:764:LEU:HG	2.15	0.46
3:F:402:ASN:O	3:F:406:LYS:HG2	2.16	0.46
3:F:9:THR:O	3:F:13:PHE:HD2	1.99	0.46
1:G:381:ILE:HA	1:G:391:THR:O	2.16	0.46
3:I:347:ASP:O	3:I:351:GLU:CB	2.62	0.46
1:J:760:ILE:O	1:J:764:LEU:HG	2.16	0.46
2:K:447:ALA:HA	2:K:450:THR:HB	1.98	0.46
3:O:231:LEU:O	3:O:235:ILE:HG12	2.16	0.46
2:Q:178:THR:HG21	2:Q:227:TYR:OH	2.15	0.46
2:Q:447:ALA:HA	2:Q:450:THR:HB	1.98	0.46
1:P:355:GLU:HA	3:R:24:ILE:HD12	1.97	0.46
1:A:626:LEU:HD11	1:A:665:ASN:HB2	1.98	0.46
2:B:137:TRP:O	2:B:141:LEU:HB2	2.16	0.46
2:B:250:GLN:HB3	2:B:267:TYR:OH	2.15	0.46
1:D:626:LEU:HD11	1:D:665:ASN:HB2	1.97	0.46
1:G:656:HIS:CD2	1:G:656:HIS:N	2.84	0.46
1:G:740:ILE:O	1:G:744:LEU:HG	2.16	0.46
1:J:362:ARG:HB3	1:J:375:PHE:HB2	1.98	0.46
1:J:427:SER:HB2	1:J:429:SER:O	2.15	0.46
1:J:573:GLU:HB3	2:K:499:LYS:HD3	1.96	0.46
1:J:740:ILE:O	1:J:744:LEU:HG	2.16	0.46
2:K:414:TYR:HE2	2:K:419:LEU:HB3	1.80	0.46
2:N:152:LEU:HA	2:N:152:LEU:HD13	1.77	0.46
3:O:141:TRP:HD1	3:O:141:TRP:H	1.58	0.46
1:P:362:ARG:HB3	1:P:375:PHE:HB2	1.98	0.46
3:R:16:ARG:NH2	3:R:183:GLU:OE2	2.49	0.46
1:A:290:GLU:HG3	1:A:291:PRO:O	2.16	0.46
1:A:446:ASP:OD1	1:A:472:ARG:HD3	2.15	0.46
1:A:662:LEU:HD13	1:A:665:ASN:CG	2.36	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:262:LEU:HD23	2:B:262:LEU:HA	1.84	0.46
1:D:740:ILE:O	1:D:744:LEU:HG	2.16	0.46
3:F:250:LEU:HD12	3:F:274:MET:HE1	1.97	0.46
3:F:362:ALA:O	3:F:365:TRP:HB2	2.17	0.46
1:G:778:ASP:CG	1:G:779:ASP:H	2.18	0.46
2:H:105:LEU:HD13	2:H:141:LEU:HD11	1.97	0.46
2:H:137:TRP:O	2:H:141:LEU:HB2	2.16	0.46
1:J:183:ASP:HB3	1:J:247:ILE:HG22	1.98	0.46
3:L:158:THR:HG23	3:L:161:ASN:H	1.81	0.46
1:M:183:ASP:HB3	1:M:247:ILE:HG22	1.98	0.46
2:N:239:PHE:HB2	2:N:245:SER:OG	2.16	0.46
2:N:96:ILE:HB	2:N:100:ALA:HB2	1.98	0.46
3:O:11:ARG:HG3	3:O:11:ARG:H	1.47	0.46
2:Q:250:GLN:OE1	2:Q:271:LYS:HD2	2.16	0.46
3:R:231:LEU:O	3:R:235:ILE:HG12	2.15	0.46
3:R:417:ILE:O	3:R:420:ASP:HB3	2.15	0.46
3:C:9:THR:O	3:C:13:PHE:HD2	1.99	0.45
1:D:183:ASP:HB3	1:D:247:ILE:HG22	1.98	0.45
1:D:573:GLU:HB3	2:E:499:LYS:HD3	1.98	0.45
2:E:108:PHE:CD1	2:E:156:LEU:HB3	2.51	0.45
3:F:16:ARG:NH2	3:F:183:GLU:OE2	2.49	0.45
1:G:746:ARG:HG2	1:G:747:LEU:N	2.30	0.45
2:H:494:SER:HB2	2:H:497:GLN:H	1.81	0.45
1:J:694:ILE:HD12	1:J:746:ARG:HG3	1.98	0.45
2:K:134:LYS:HA	2:K:134:LYS:HD3	1.78	0.45
2:K:136:ILE:HG12	2:K:243:PHE:CZ	2.51	0.45
2:K:435:GLN:H	2:K:435:GLN:HG3	1.41	0.45
3:L:16:ARG:NH2	3:L:183:GLU:OE2	2.49	0.45
1:M:60:VAL:O	1:M:61:VAL:HG23	2.16	0.45
1:M:757:GLN:HE21	1:M:758:ASN:N	2.14	0.45
2:N:137:TRP:HE3	2:N:140:ILE:HD11	1.81	0.45
1:P:353:ASP:OD2	1:P:355:GLU:HG3	2.16	0.45
1:P:626:LEU:HD22	1:P:626:LEU:HA	1.65	0.45
2:Q:250:GLN:HB3	2:Q:267:TYR:OH	2.16	0.45
3:R:82:ARG:HD2	3:R:82:ARG:O	2.16	0.45
1:D:290:GLU:HG3	1:D:291:PRO:O	2.17	0.45
1:D:626:LEU:HA	1:D:626:LEU:HD22	1.64	0.45
1:G:353:ASP:OD2	1:G:355:GLU:HG3	2.16	0.45
1:G:573:GLU:HB3	2:H:499:LYS:HD3	1.97	0.45
2:H:178:THR:HG21	2:H:227:TYR:OH	2.16	0.45
2:H:250:GLN:OE1	2:H:271:LYS:HD2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:386:LEU:HD13	3:I:241:ARG:NH2	2.31	0.45
1:J:425:GLY:O	1:J:426:ALA:HB2	2.16	0.45
3:L:82:ARG:HD2	3:L:82:ARG:O	2.16	0.45
1:M:362:ARG:HB3	1:M:375:PHE:HB2	1.98	0.45
2:N:137:TRP:CH2	2:N:141:LEU:HD13	2.51	0.45
2:N:250:GLN:OE1	2:N:271:LYS:HD2	2.17	0.45
3:R:295:PRO:HB3	3:R:296:PRO:HD2	1.96	0.45
1:A:421:ILE:CG2	1:A:423:ILE:HG13	2.46	0.45
1:A:599:LYS:HG2	2:B:272:GLN:OE1	2.16	0.45
3:C:82:ARG:HD2	3:C:82:ARG:O	2.16	0.45
2:E:137:TRP:O	2:E:141:LEU:HB2	2.16	0.45
2:E:314:ILE:O	2:E:318:LEU:HB2	2.16	0.45
1:G:656:HIS:HB2	1:G:748:GLU:HA	1.98	0.45
1:G:760:ILE:O	1:G:764:LEU:HG	2.16	0.45
2:H:108:PHE:CD1	2:H:156:LEU:HB3	2.51	0.45
3:I:173:MET:O	3:I:176:PRO:HD2	2.17	0.45
3:I:16:ARG:NH2	3:I:183:GLU:OE2	2.49	0.45
1:J:389:TRP:HH2	3:L:147:GLN:HA	1.81	0.45
1:M:425:GLY:O	1:M:426:ALA:HB2	2.16	0.45
2:N:136:ILE:HG12	2:N:243:PHE:CZ	2.52	0.45
3:O:250:LEU:HD12	3:O:274:MET:HE1	1.97	0.45
1:P:740:ILE:O	1:P:744:LEU:HG	2.17	0.45
2:Q:136:ILE:HG12	2:Q:243:PHE:CZ	2.51	0.45
2:Q:289:ARG:O	2:Q:289:ARG:HG3	2.17	0.45
2:Q:494:SER:HB2	2:Q:497:GLN:H	1.81	0.45
2:Q:512:ARG:HD3	2:Q:512:ARG:HA	1.83	0.45
3:R:250:LEU:HD12	3:R:274:MET:HE1	1.98	0.45
3:F:302:ARG:H	3:F:302:ARG:HG2	1.45	0.45
1:G:290:GLU:HG3	1:G:291:PRO:O	2.16	0.45
2:H:252:LEU:O	2:H:256:LEU:HB2	2.17	0.45
3:I:158:THR:HG23	3:I:161:ASN:H	1.82	0.45
1:J:381:ILE:HA	1:J:391:THR:O	2.15	0.45
1:J:60:VAL:O	1:J:61:VAL:HG23	2.16	0.45
1:J:650:LEU:HD22	2:K:242:PHE:HA	1.98	0.45
1:J:656:HIS:N	1:J:656:HIS:CD2	2.84	0.45
2:K:252:LEU:O	2:K:256:LEU:HB2	2.17	0.45
2:B:444:GLU:HG2	3:L:171:ARG:HH22	1.80	0.45
3:L:362:ALA:O	3:L:365:TRP:HB2	2.16	0.45
1:M:353:ASP:OD2	1:M:355:GLU:HG3	2.16	0.45
2:N:105:LEU:HD13	2:N:141:LEU:HD11	1.98	0.45
3:O:402:ASN:O	3:O:406:LYS:HG2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:105:LEU:HD13	2:Q:141:LEU:HD11	1.97	0.45
2:Q:502:ILE:HA	2:Q:505:ILE:HG22	1.96	0.45
2:B:252:LEU:O	2:B:256:LEU:HB2	2.17	0.45
1:G:441:ASP:HA	1:G:442:LEU:HD13	1.99	0.45
2:H:152:LEU:HD12	2:H:154:LEU:HD11	1.99	0.45
3:I:141:TRP:HD1	3:I:141:TRP:H	1.58	0.45
2:K:221:PRO:HD2	2:K:222:PHE:CD2	2.52	0.45
3:L:9:THR:O	3:L:13:PHE:HD2	1.99	0.45
1:M:626:LEU:HA	1:M:626:LEU:HD22	1.65	0.45
3:O:82:ARG:HD2	3:O:82:ARG:O	2.17	0.45
2:Q:138:LEU:HD23	2:Q:138:LEU:HA	1.84	0.45
3:R:11:ARG:H	3:R:11:ARG:HG3	1.48	0.45
1:A:760:ILE:O	1:A:764:LEU:HG	2.16	0.45
3:C:171:ARG:C	3:C:174:GLU:H	2.20	0.45
3:C:234:LYS:O	3:C:238:THR:OG1	2.34	0.45
1:G:425:GLY:O	1:G:426:ALA:HB2	2.17	0.45
1:G:757:GLN:HE21	1:G:758:ASN:N	2.14	0.45
3:I:402:ASN:O	3:I:406:LYS:HG2	2.16	0.45
1:J:425:GLY:HA2	1:J:435:ARG:HB2	1.97	0.45
1:J:746:ARG:HG2	1:J:747:LEU:N	2.31	0.45
1:M:760:ILE:O	1:M:764:LEU:HG	2.16	0.45
3:O:158:THR:HG23	3:O:161:ASN:H	1.80	0.45
3:O:9:THR:O	3:O:13:PHE:HD2	2.00	0.45
1:P:441:ASP:HA	1:P:442:LEU:HD13	1.99	0.45
1:P:619:GLU:OE2	1:P:670:ALA:N	2.50	0.45
1:P:760:ILE:O	1:P:764:LEU:HG	2.15	0.45
1:A:660:LYS:HA	1:A:660:LYS:HD3	1.66	0.45
1:A:619:GLU:OE2	1:A:670:ALA:N	2.49	0.45
2:B:96:ILE:HB	2:B:100:ALA:HB2	1.99	0.45
1:D:353:ASP:OD2	1:D:355:GLU:HG3	2.17	0.45
1:D:441:ASP:HA	1:D:442:LEU:HD13	1.99	0.45
1:D:452:THR:HG21	1:D:508:ILE:HG22	1.99	0.45
1:D:778:ASP:CG	1:D:779:ASP:H	2.18	0.45
2:E:136:ILE:HG12	2:E:243:PHE:CZ	2.52	0.45
2:E:239:PHE:HB2	2:E:245:SER:OG	2.17	0.45
3:F:231:LEU:O	3:F:235:ILE:HG12	2.17	0.45
2:E:386:LEU:HD13	3:F:241:ARG:NH2	2.32	0.45
1:G:265:THR:OG1	1:G:268:SER:N	2.41	0.45
1:G:273:ARG:HH11	1:G:273:ARG:H	1.64	0.45
1:G:323:ASN:N	1:G:323:ASN:OD1	2.50	0.45
1:G:694:ILE:HD12	1:G:746:ARG:HG3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:291:ASP:OD2	2:H:291:ASP:N	2.50	0.45
3:I:362:ALA:O	3:I:365:TRP:HB2	2.17	0.45
1:J:470:SER:O	1:J:504:THR:HG22	2.16	0.45
1:M:323:ASN:N	1:M:323:ASN:OD1	2.49	0.45
1:M:427:SER:HB2	1:M:429:SER:O	2.16	0.45
2:N:181:TYR:O	2:N:185:ILE:HG12	2.16	0.45
2:N:221:PRO:HD2	2:N:222:PHE:CD2	2.51	0.45
1:P:637:LEU:HA	1:P:637:LEU:HD22	1.81	0.45
2:Q:221:PRO:HD2	2:Q:222:PHE:CD2	2.52	0.45
2:Q:291:ASP:OD2	2:Q:291:ASP:N	2.50	0.45
3:R:9:THR:O	3:R:13:PHE:HD2	2.00	0.45
2:B:140:ILE:HG22	2:B:236:MET:HG2	1.99	0.45
2:B:250:GLN:OE1	2:B:271:LYS:HD2	2.16	0.45
2:B:495:LYS:CG	2:B:499:LYS:HZ1	2.30	0.45
1:A:573:GLU:HB3	2:B:499:LYS:HD3	1.98	0.45
3:C:347:ASP:O	3:C:351:GLU:CB	2.61	0.45
3:C:402:ASN:O	3:C:405:ILE:HB	2.17	0.45
1:D:656:HIS:HB2	1:D:748:GLU:HA	1.99	0.45
2:E:152:LEU:HD12	2:E:154:LEU:HD11	1.99	0.45
2:H:239:PHE:HB2	2:H:245:SER:OG	2.17	0.45
1:J:323:ASN:OD1	1:J:323:ASN:N	2.50	0.45
1:J:599:LYS:HG2	2:K:272:GLN:OE1	2.16	0.45
1:M:381:ILE:HA	1:M:391:THR:O	2.16	0.45
1:P:656:HIS:HB2	1:P:748:GLU:HA	1.99	0.45
1:A:353:ASP:OD2	1:A:355:GLU:HG3	2.16	0.45
1:A:394:VAL:HG21	3:C:143:THR:HG22	1.98	0.45
3:C:168:ILE:HD11	3:C:172:LYS:HE2	1.99	0.45
1:D:362:ARG:HB3	1:D:375:PHE:HB2	1.99	0.45
2:E:291:ASP:OD2	2:E:291:ASP:N	2.49	0.45
3:F:158:THR:HG23	3:F:161:ASN:H	1.81	0.45
1:G:319:ASP:HB2	1:G:363:ILE:CG1	2.47	0.45
1:G:637:LEU:HD22	1:G:637:LEU:HA	1.82	0.45
2:H:136:ILE:HG12	2:H:243:PHE:CZ	2.52	0.45
1:J:273:ARG:HH11	1:J:273:ARG:H	1.64	0.45
1:J:656:HIS:HB2	1:J:748:GLU:HA	1.99	0.45
2:K:250:GLN:OE1	2:K:271:LYS:HD2	2.16	0.45
2:K:314:ILE:O	2:K:318:LEU:HB2	2.17	0.45
2:K:408:ILE:HD11	2:K:412:LYS:HE3	1.99	0.45
3:L:15:GLN:HA	3:L:18:LYS:HE2	1.98	0.45
3:L:291:ARG:HG2	3:L:292:SER:H	1.82	0.45
3:L:402:ASN:O	3:L:405:ILE:HB	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:289:ARG:HG3	2:N:289:ARG:O	2.17	0.45
3:O:173:MET:O	3:O:176:PRO:HD2	2.17	0.45
1:P:273:ARG:H	1:P:273:ARG:HH11	1.64	0.45
1:P:384:ASP:CB	1:P:389:TRP:HB3	2.46	0.45
1:P:659:LEU:H	1:P:659:LEU:CD1	2.29	0.45
2:Q:239:PHE:CG	2:Q:240:LYS:N	2.84	0.45
1:A:273:ARG:H	1:A:273:ARG:HH11	1.64	0.45
1:A:441:ASP:HA	1:A:442:LEU:HD13	1.99	0.45
1:A:60:VAL:O	1:A:61:VAL:HG23	2.17	0.45
2:B:239:PHE:HB2	2:B:245:SER:OG	2.17	0.45
3:C:11:ARG:H	3:C:11:ARG:HG3	1.48	0.45
3:C:303:THR:HA	3:C:358:PHE:HZ	1.82	0.45
2:E:290:THR:HB	2:E:292:GLU:N	2.31	0.45
2:E:484:ALA:O	2:E:488:LEU:HG	2.16	0.45
1:G:207:SER:O	1:G:213:VAL:HG22	2.17	0.45
2:H:137:TRP:HE3	2:H:140:ILE:HD11	1.81	0.45
2:H:153:LYS:HB3	2:H:153:LYS:HE2	1.78	0.45
2:H:314:ILE:O	2:H:318:LEU:HB2	2.17	0.45
3:I:82:ARG:HD2	3:I:82:ARG:O	2.17	0.45
1:J:270:GLN:HG2	1:J:291:PRO:HB3	1.99	0.45
1:J:319:ASP:HB2	1:J:363:ILE:CG1	2.47	0.45
2:K:291:ASP:N	2:K:291:ASP:OD2	2.50	0.45
1:M:441:ASP:HA	1:M:442:LEU:HD13	1.99	0.45
2:N:178:THR:HG21	2:N:227:TYR:OH	2.16	0.45
2:N:447:ALA:HA	2:N:450:THR:HB	1.98	0.45
3:O:308:PHE:HD1	3:O:309:ALA:H	1.65	0.45
3:O:312:TYR:O	3:O:316:SER:OG	2.22	0.45
1:P:470:SER:O	1:P:504:THR:HG22	2.17	0.45
2:Q:137:TRP:HE3	2:Q:140:ILE:HD11	1.82	0.45
2:Q:152:LEU:HB3	2:Q:154:LEU:CD2	2.47	0.45
2:Q:495:LYS:CG	2:Q:499:LYS:HZ1	2.30	0.45
1:A:425:GLY:O	1:A:426:ALA:HB2	2.17	0.44
2:B:239:PHE:CG	2:B:240:LYS:N	2.85	0.44
1:D:273:ARG:H	1:D:273:ARG:HH11	1.64	0.44
2:E:105:LEU:HD13	2:E:141:LEU:HD11	1.98	0.44
2:E:495:LYS:CG	2:E:499:LYS:HZ1	2.31	0.44
1:G:389:TRP:HH2	3:I:147:GLN:HA	1.82	0.44
2:H:118:TRP:CZ2	2:H:189:LYS:HB3	2.52	0.44
2:H:239:PHE:CG	2:H:240:LYS:N	2.85	0.44
3:I:402:ASN:O	3:I:405:ILE:HB	2.17	0.44
1:J:353:ASP:OD2	1:J:355:GLU:HG3	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:234:CYS:SG	2:K:284:LEU:HB3	2.58	0.44
1:M:265:THR:HG1	1:M:268:SER:H	1.64	0.44
1:M:694:ILE:HD12	1:M:746:ARG:HG3	1.98	0.44
3:O:168:ILE:HD11	3:O:172:LYS:HE2	1.99	0.44
3:O:402:ASN:O	3:O:405:ILE:HB	2.16	0.44
1:P:290:GLU:HG3	1:P:291:PRO:O	2.17	0.44
1:P:270:GLN:HG2	1:P:291:PRO:HB3	1.99	0.44
1:P:425:GLY:O	1:P:426:ALA:HB2	2.17	0.44
2:Q:137:TRP:O	2:Q:141:LEU:HB2	2.16	0.44
2:Q:332:LEU:HA	2:Q:332:LEU:HD13	1.78	0.44
1:A:265:THR:OG1	1:A:268:SER:N	2.42	0.44
1:A:270:GLN:HG2	1:A:291:PRO:HB3	1.99	0.44
2:B:289:ARG:HG3	2:B:289:ARG:O	2.17	0.44
2:E:494:SER:HB2	2:E:497:GLN:H	1.81	0.44
1:G:270:GLN:HG2	1:G:291:PRO:HB3	1.99	0.44
3:I:303:THR:HA	3:I:358:PHE:HZ	1.82	0.44
1:J:218:VAL:HG23	1:J:228:ASN:ND2	2.32	0.44
2:K:239:PHE:CG	2:K:240:LYS:N	2.85	0.44
1:M:421:ILE:CG2	1:M:423:ILE:HG13	2.47	0.44
3:O:421:LYS:HG3	3:O:422:GLY:N	2.32	0.44
1:P:183:ASP:HB3	1:P:247:ILE:HG22	1.99	0.44
1:P:452:THR:HG21	1:P:508:ILE:HG22	1.99	0.44
2:Q:108:PHE:CD1	2:Q:156:LEU:HB3	2.51	0.44
2:Q:152:LEU:HD12	2:Q:154:LEU:HD11	1.99	0.44
3:R:152:ILE:HG13	3:R:153:ASN:H	1.82	0.44
3:R:27:ILE:HD11	3:R:166:GLU:HA	2.00	0.44
2:B:291:ASP:OD2	2:B:291:ASP:N	2.50	0.44
1:D:377:ARG:NH2	1:D:378:SER:OG	2.35	0.44
2:E:252:LEU:O	2:E:256:LEU:HB2	2.18	0.44
2:E:435:GLN:H	2:E:435:GLN:HG3	1.42	0.44
1:G:369:PHE:HD1	1:G:369:PHE:O	2.01	0.44
2:H:178:THR:HG22	2:H:303:GLU:OE1	2.18	0.44
2:H:221:PRO:HD2	2:H:222:PHE:CD2	2.52	0.44
1:J:207:SER:O	1:J:213:VAL:HG22	2.17	0.44
1:J:441:ASP:HA	1:J:442:LEU:HD13	2.00	0.44
2:K:494:SER:HB2	2:K:497:GLN:H	1.82	0.44
3:O:303:THR:HA	3:O:358:PHE:HZ	1.82	0.44
1:P:492:LEU:HD22	1:P:492:LEU:H	1.83	0.44
1:P:60:VAL:O	1:P:61:VAL:HG23	2.18	0.44
1:P:675:PHE:HZ	1:P:742:TRP:HZ3	1.65	0.44
2:Q:408:ILE:HD11	2:Q:412:LYS:HE3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:R:362:ALA:O	3:R:365:TRP:HB2	2.17	0.44
3:R:402:ASN:O	3:R:405:ILE:HB	2.16	0.44
1:A:207:SER:O	1:A:213:VAL:HG22	2.17	0.44
1:A:492:LEU:H	1:A:492:LEU:HD22	1.82	0.44
1:A:739:ASP:OD1	2:B:250:GLN:NE2	2.50	0.44
2:B:194:GLN:HG3	3:C:209:ARG:HH11	1.83	0.44
1:D:425:GLY:O	1:D:426:ALA:HB2	2.17	0.44
2:E:181:TYR:O	2:E:185:ILE:HG12	2.18	0.44
2:E:289:ARG:O	2:E:289:ARG:HG3	2.17	0.44
1:G:245:ILE:HG23	1:G:263:ILE:HG22	1.99	0.44
1:G:421:ILE:CG2	1:G:423:ILE:HG13	2.47	0.44
3:I:171:ARG:HH22	2:K:444:GLU:HG2	1.82	0.44
1:J:626:LEU:HA	1:J:626:LEU:HD22	1.65	0.44
1:J:697:GLU:HG2	1:J:698:LYS:H	1.83	0.44
2:K:137:TRP:HE3	2:K:140:ILE:HD11	1.82	0.44
3:L:250:LEU:HB2	3:L:270:PHE:CE2	2.51	0.44
2:N:408:ILE:HD11	2:N:412:LYS:HE3	2.00	0.44
1:P:207:SER:O	1:P:213:VAL:HG22	2.18	0.44
1:P:319:ASP:HB2	1:P:363:ILE:CG1	2.47	0.44
1:A:323:ASN:N	1:A:323:ASN:OD1	2.49	0.44
1:A:427:SER:HB2	1:A:429:SER:O	2.16	0.44
1:G:394:VAL:HG21	3:I:143:THR:HG22	1.99	0.44
2:H:289:ARG:HG3	2:H:289:ARG:O	2.17	0.44
1:J:290:GLU:HG3	1:J:291:PRO:O	2.17	0.44
1:J:421:ILE:CG2	1:J:423:ILE:HG13	2.48	0.44
2:K:118:TRP:CZ2	2:K:189:LYS:HB3	2.52	0.44
3:L:171:ARG:C	3:L:174:GLU:H	2.21	0.44
2:N:108:PHE:CD1	2:N:156:LEU:HB3	2.51	0.44
2:N:239:PHE:CG	2:N:240:LYS:N	2.84	0.44
3:O:250:LEU:HB2	3:O:270:PHE:CE2	2.50	0.44
1:A:319:ASP:HB2	1:A:363:ILE:CG1	2.47	0.44
1:A:369:PHE:HD1	1:A:369:PHE:O	2.01	0.44
1:A:694:ILE:HD12	1:A:746:ARG:HG3	1.98	0.44
2:B:118:TRP:CZ2	2:B:189:LYS:HB3	2.52	0.44
2:B:408:ILE:HD11	2:B:412:LYS:HE3	2.00	0.44
3:C:362:ALA:O	3:C:365:TRP:HB2	2.17	0.44
3:C:421:LYS:HG3	3:C:422:GLY:N	2.32	0.44
1:D:207:SER:O	1:D:213:VAL:HG22	2.18	0.44
1:D:421:ILE:CG2	1:D:423:ILE:HG13	2.47	0.44
2:E:137:TRP:HE3	2:E:140:ILE:HD11	1.82	0.44
2:E:178:THR:HG22	2:E:303:GLU:OE1	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:239:PHE:CG	2:E:240:LYS:N	2.85	0.44
3:F:308:PHE:HD1	3:F:309:ALA:H	1.66	0.44
3:F:313:LEU:HA	3:F:313:LEU:HD12	1.87	0.44
1:G:361:LYS:HA	1:G:375:PHE:O	2.18	0.44
1:G:681:GLN:HA	1:G:684:GLN:HB2	2.00	0.44
1:G:739:ASP:OD1	2:H:250:GLN:NE2	2.51	0.44
3:I:291:ARG:HG2	3:I:292:SER:H	1.83	0.44
3:I:308:PHE:HD1	3:I:309:ALA:H	1.66	0.44
2:K:108:PHE:CD1	2:K:156:LEU:HB3	2.52	0.44
3:L:152:ILE:HG13	3:L:153:ASN:H	1.82	0.44
1:M:290:GLU:HG3	1:M:291:PRO:O	2.17	0.44
1:M:611:ILE:CD1	1:M:731:LEU:HB2	2.48	0.44
3:O:312:TYR:HA	3:O:315:SER:HG	1.83	0.44
1:P:369:PHE:O	1:P:369:PHE:HD1	2.01	0.44
2:Q:118:TRP:CZ2	2:Q:189:LYS:HB3	2.52	0.44
2:Q:239:PHE:HB2	2:Q:245:SER:OG	2.17	0.44
3:R:173:MET:O	3:R:176:PRO:HD2	2.18	0.44
1:A:245:ILE:HG23	1:A:263:ILE:HG22	1.99	0.44
2:B:178:THR:HG21	2:B:227:TYR:OH	2.18	0.44
2:B:221:PRO:HD2	2:B:222:PHE:CD2	2.52	0.44
3:F:235:ILE:HG12	3:F:235:ILE:H	1.60	0.44
3:F:236:PHE:CE2	3:F:253:ILE:HD12	2.52	0.44
3:F:27:ILE:HD11	3:F:166:GLU:HA	2.00	0.44
2:H:447:ALA:HA	2:H:450:THR:HB	1.98	0.44
1:G:574:TRP:CH2	2:H:495:LYS:HD2	2.52	0.44
2:H:96:ILE:HB	2:H:100:ALA:HB2	1.99	0.44
3:I:15:GLN:HA	3:I:18:LYS:HE2	1.99	0.44
1:J:417:THR:OG1	1:J:451:ILE:HB	2.18	0.44
2:K:152:LEU:HD12	2:K:154:LEU:HD11	2.00	0.44
1:J:739:ASP:OD1	2:K:250:GLN:NE2	2.51	0.44
2:K:289:ARG:O	2:K:289:ARG:HG3	2.17	0.44
3:L:312:TYR:HA	3:L:315:SER:HG	1.83	0.44
3:L:303:THR:HA	3:L:358:PHE:HZ	1.82	0.44
1:M:270:GLN:HG2	1:M:291:PRO:HB3	1.99	0.44
2:N:152:LEU:HB3	2:N:154:LEU:CD2	2.47	0.44
2:N:366:TYR:HA	2:N:369:TRP:CD1	2.52	0.44
2:Q:290:THR:HB	2:Q:292:GLU:N	2.31	0.44
1:A:681:GLN:HA	1:A:684:GLN:HB2	2.00	0.44
1:A:690:ASP:OD1	1:A:750:PRO:HB3	2.18	0.44
3:C:291:ARG:HG2	3:C:292:SER:H	1.83	0.44
1:D:319:ASP:HB2	1:D:363:ILE:CG1	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:369:PHE:HD1	1:D:369:PHE:O	2.01	0.44
1:D:389:TRP:HH2	3:F:147:GLN:HA	1.81	0.44
1:D:492:LEU:HD22	1:D:492:LEU:H	1.83	0.44
2:E:129:PHE:HE1	2:E:169:SER:N	2.16	0.44
2:E:96:ILE:HB	2:E:100:ALA:HB2	1.99	0.44
1:G:301:GLN:CD	1:G:360:TRP:HA	2.38	0.44
1:G:492:LEU:H	1:G:492:LEU:HD22	1.81	0.44
3:I:421:LYS:HG3	3:I:422:GLY:N	2.33	0.44
1:J:443:ASP:O	3:L:3:GLU:N	2.50	0.44
1:M:273:ARG:H	1:M:273:ARG:HH11	1.64	0.44
1:M:384:ASP:CB	1:M:389:TRP:HB3	2.46	0.44
1:M:697:GLU:HG2	1:M:698:LYS:H	1.83	0.44
1:P:245:ILE:HG23	1:P:263:ILE:HG22	1.98	0.44
2:Q:366:TYR:HA	2:Q:369:TRP:CD1	2.53	0.44
2:Q:439:ILE:H	2:Q:439:ILE:HG13	1.66	0.44
3:R:8:LEU:HD22	3:R:8:LEU:H	1.82	0.44
1:A:626:LEU:HD22	1:A:626:LEU:HA	1.65	0.44
3:F:291:ARG:HG2	3:F:292:SER:H	1.83	0.44
1:G:632:ILE:O	1:G:636:GLU:HG3	2.18	0.44
2:H:290:THR:HB	2:H:292:GLU:N	2.31	0.44
1:M:319:ASP:HB2	1:M:363:ILE:CG1	2.47	0.44
1:M:452:THR:HG21	1:M:508:ILE:HG22	1.99	0.44
1:M:675:PHE:HZ	1:M:742:TRP:HZ3	1.66	0.44
1:M:762:ARG:HE	1:M:762:ARG:HA	1.83	0.44
3:O:165:ILE:HG13	3:O:165:ILE:H	1.68	0.44
3:O:427:PRO:HD3	3:O:430:LEU:HB2	2.00	0.44
1:P:218:VAL:HG23	1:P:228:ASN:ND2	2.33	0.44
1:A:274:ILE:HD13	1:A:286:VAL:HB	2.00	0.43
1:A:675:PHE:HZ	1:A:742:TRP:HZ3	1.66	0.43
3:C:430:LEU:HD13	3:C:430:LEU:HA	1.85	0.43
2:E:118:TRP:CZ2	2:E:189:LYS:HB3	2.53	0.43
2:E:255:LYS:O	2:E:259:GLN:HB2	2.18	0.43
3:F:402:ASN:O	3:F:405:ILE:HB	2.17	0.43
1:G:377:ARG:NH2	1:G:378:SER:OG	2.34	0.43
2:H:138:LEU:HD23	2:H:138:LEU:HA	1.85	0.43
2:H:408:ILE:HD11	2:H:412:LYS:HE3	2.00	0.43
2:H:495:LYS:HE2	2:H:499:LYS:NZ	2.33	0.43
1:J:369:PHE:HD1	1:J:369:PHE:O	2.01	0.43
1:J:681:GLN:HA	1:J:684:GLN:HB2	2.00	0.43
1:J:690:ASP:OD1	1:J:750:PRO:HB3	2.18	0.43
1:M:470:SER:O	1:M:504:THR:HG22	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:291:ASP:N	2:N:291:ASP:OD2	2.50	0.43
2:N:495:LYS:HE2	2:N:499:LYS:NZ	2.33	0.43
1:M:394:VAL:HG21	3:O:143:THR:HG22	1.99	0.43
3:O:27:ILE:HD11	3:O:166:GLU:HA	2.00	0.43
3:R:303:THR:HA	3:R:358:PHE:HZ	1.82	0.43
3:C:1:MET:HG3	3:C:2:PHE:CD1	2.53	0.43
1:D:470:SER:O	1:D:504:THR:HG22	2.17	0.43
1:D:681:GLN:HA	1:D:684:GLN:HB2	2.01	0.43
1:D:697:GLU:HG2	1:D:698:LYS:H	1.83	0.43
2:E:152:LEU:HB3	2:E:154:LEU:CD2	2.47	0.43
2:E:495:LYS:HE2	2:E:499:LYS:NZ	2.33	0.43
3:F:173:MET:O	3:F:176:PRO:HD2	2.18	0.43
3:F:303:THR:HA	3:F:358:PHE:HZ	1.83	0.43
1:D:443:ASP:O	3:F:3:GLU:N	2.51	0.43
2:H:129:PHE:HE1	2:H:169:SER:N	2.17	0.43
3:I:152:ILE:HG13	3:I:153:ASN:H	1.83	0.43
3:I:236:PHE:CE2	3:I:253:ILE:HD12	2.53	0.43
2:K:129:PHE:HE1	2:K:169:SER:N	2.16	0.43
2:K:152:LEU:HD13	2:K:152:LEU:HA	1.77	0.43
2:K:255:LYS:O	2:K:259:GLN:HB2	2.18	0.43
1:M:369:PHE:HD1	1:M:369:PHE:O	2.01	0.43
2:N:118:TRP:CZ2	2:N:189:LYS:HB3	2.53	0.43
2:N:314:ILE:O	2:N:318:LEU:HB2	2.17	0.43
2:N:318:LEU:HD12	2:N:318:LEU:HA	1.82	0.43
1:P:632:ILE:O	1:P:636:GLU:HG3	2.19	0.43
2:Q:129:PHE:HE1	2:Q:169:SER:N	2.16	0.43
2:Q:152:LEU:HA	2:Q:152:LEU:HD13	1.77	0.43
3:R:168:ILE:HD11	3:R:172:LYS:HE2	2.00	0.43
3:R:435:LEU:O	3:R:439:GLU:HG3	2.18	0.43
1:A:218:VAL:HG23	1:A:228:ASN:ND2	2.33	0.43
1:A:656:HIS:HB2	1:A:748:GLU:HA	1.99	0.43
2:E:221:PRO:HD2	2:E:222:PHE:CD2	2.53	0.43
1:D:739:ASP:OD1	2:E:250:GLN:NE2	2.51	0.43
1:G:413:GLY:HA2	1:G:426:ALA:HB2	2.01	0.43
1:G:626:LEU:HD11	1:G:665:ASN:HB2	1.99	0.43
1:G:697:GLU:HG2	1:G:698:LYS:H	1.83	0.43
2:H:194:GLN:HG3	3:I:209:ARG:HH11	1.83	0.43
3:L:421:LYS:HG3	3:L:422:GLY:N	2.33	0.43
2:N:332:LEU:HA	2:N:332:LEU:HD13	1.80	0.43
3:O:347:ASP:O	3:O:351:GLU:CB	2.61	0.43
1:P:361:LYS:HA	1:P:375:PHE:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:681:GLN:HA	1:P:684:GLN:HB2	2.00	0.43
2:Q:96:ILE:HB	2:Q:100:ALA:HB2	1.99	0.43
3:R:308:PHE:HD1	3:R:309:ALA:H	1.67	0.43
2:B:137:TRP:HE3	2:B:140:ILE:HD11	1.83	0.43
2:B:181:TYR:O	2:B:185:ILE:HG12	2.18	0.43
3:C:235:ILE:HG12	3:C:235:ILE:H	1.60	0.43
1:D:632:ILE:O	1:D:636:GLU:HG3	2.18	0.43
2:E:381:MET:O	2:E:385:PHE:HB2	2.19	0.43
3:F:152:ILE:HG13	3:F:153:ASN:H	1.83	0.43
1:G:452:THR:HG21	1:G:508:ILE:HG22	2.00	0.43
1:G:690:ASP:OD1	1:G:750:PRO:HB3	2.18	0.43
2:H:419:LEU:HD13	2:H:419:LEU:H	1.83	0.43
3:I:171:ARG:C	3:I:174:GLU:H	2.22	0.43
1:J:762:ARG:HE	1:J:762:ARG:HA	1.83	0.43
3:L:235:ILE:HG12	3:L:235:ILE:H	1.59	0.43
1:M:245:ILE:HG23	1:M:263:ILE:HG22	1.99	0.43
1:M:681:GLN:HA	1:M:684:GLN:HB2	2.00	0.43
1:M:753:PHE:HA	1:M:753:PHE:HD1	1.65	0.43
2:N:152:LEU:HD12	2:N:154:LEU:HD11	2.00	0.43
3:O:171:ARG:C	3:O:174:GLU:H	2.22	0.43
3:O:291:ARG:HG2	3:O:292:SER:H	1.83	0.43
3:O:362:ALA:O	3:O:365:TRP:HB2	2.17	0.43
1:P:274:ILE:HD13	1:P:286:VAL:HB	2.00	0.43
1:P:697:GLU:HG2	1:P:698:LYS:H	1.84	0.43
2:Q:419:LEU:H	2:Q:419:LEU:HD13	1.83	0.43
3:R:141:TRP:H	3:R:141:TRP:HD1	1.58	0.43
1:P:394:VAL:HG21	3:R:143:THR:HG22	2.00	0.43
1:A:265:THR:HG1	1:A:268:SER:H	1.66	0.43
1:A:632:ILE:O	1:A:636:GLU:HG3	2.19	0.43
1:A:762:ARG:HE	1:A:762:ARG:HA	1.84	0.43
2:B:108:PHE:CE1	2:B:156:LEU:HB3	2.54	0.43
2:B:152:LEU:HA	2:B:152:LEU:HD13	1.77	0.43
1:D:245:ILE:HG23	1:D:263:ILE:HG22	1.99	0.43
1:D:314:GLN:HA	1:D:314:GLN:OE1	2.19	0.43
2:E:419:LEU:HD13	2:E:419:LEU:H	1.83	0.43
3:F:82:ARG:O	3:F:82:ARG:HD2	2.17	0.43
1:G:412:ASN:O	1:G:426:ALA:HB1	2.19	0.43
1:G:60:VAL:O	1:G:61:VAL:HG23	2.17	0.43
1:G:762:ARG:HB3	2:H:138:LEU:HD13	2.01	0.43
2:H:140:ILE:HG22	2:H:236:MET:HG2	2.01	0.43
3:I:312:TYR:HA	3:I:315:SER:HG	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:8:LEU:H	3:I:8:LEU:HD22	1.82	0.43
1:J:452:THR:HG21	1:J:508:ILE:HG22	2.00	0.43
1:J:675:PHE:HZ	1:J:742:TRP:HZ3	1.67	0.43
2:K:140:ILE:HG22	2:K:236:MET:HG2	2.00	0.43
2:K:366:TYR:HA	2:K:369:TRP:CD1	2.53	0.43
3:L:173:MET:O	3:L:176:PRO:HD2	2.18	0.43
1:M:492:LEU:H	1:M:492:LEU:HD22	1.83	0.43
2:N:137:TRP:O	2:N:141:LEU:HB2	2.18	0.43
2:N:381:MET:O	2:N:385:PHE:HB2	2.19	0.43
1:P:690:ASP:OD1	1:P:750:PRO:HB3	2.17	0.43
2:B:484:ALA:O	2:B:488:LEU:HG	2.18	0.43
3:C:308:PHE:HD1	3:C:309:ALA:H	1.67	0.43
3:C:427:PRO:HD3	3:C:430:LEU:HB2	2.00	0.43
1:D:270:GLN:HG2	1:D:291:PRO:HB3	2.00	0.43
1:D:532:GLU:HB2	1:D:554:ASN:CB	2.49	0.43
3:F:141:TRP:H	3:F:141:TRP:HD1	1.58	0.43
3:F:80:ARG:O	3:F:83:HIS:HB3	2.19	0.43
1:G:675:PHE:HZ	1:G:742:TRP:HZ3	1.66	0.43
3:I:235:ILE:HG12	3:I:235:ILE:H	1.59	0.43
3:L:427:PRO:HD3	3:L:430:LEU:HB2	1.99	0.43
1:M:362:ARG:NH2	1:M:364:GLU:HG3	2.33	0.43
1:M:656:HIS:CD2	1:M:656:HIS:N	2.84	0.43
1:M:656:HIS:HB2	1:M:748:GLU:HA	1.99	0.43
2:N:129:PHE:HE1	2:N:169:SER:N	2.16	0.43
3:O:152:ILE:HG13	3:O:153:ASN:H	1.82	0.43
1:P:532:GLU:HB2	1:P:554:ASN:CB	2.49	0.43
2:Q:108:PHE:CE1	2:Q:156:LEU:HB3	2.53	0.43
2:Q:181:TYR:O	2:Q:185:ILE:HG12	2.19	0.43
3:R:427:PRO:HD3	3:R:430:LEU:HB2	2.00	0.43
1:A:361:LYS:HA	1:A:375:PHE:O	2.19	0.43
1:A:384:ASP:CB	1:A:389:TRP:HB3	2.46	0.43
2:B:178:THR:HG22	2:B:303:GLU:OE1	2.18	0.43
2:B:381:MET:O	2:B:385:PHE:HB2	2.18	0.43
3:C:152:ILE:HG13	3:C:153:ASN:H	1.83	0.43
1:D:301:GLN:CD	1:D:360:TRP:HA	2.39	0.43
1:D:408:ILE:HG23	1:D:414:ILE:N	2.34	0.43
2:E:262:LEU:HA	2:E:262:LEU:HD23	1.85	0.43
2:E:250:GLN:OE1	2:E:271:LYS:HD2	2.17	0.43
2:E:194:GLN:HG3	3:F:209:ARG:NH1	2.34	0.43
1:G:218:VAL:HG23	1:G:228:ASN:ND2	2.33	0.43
1:G:363:ILE:O	1:G:363:ILE:HD12	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:470:SER:O	1:G:504:THR:HG22	2.18	0.43
2:H:152:LEU:HB3	2:H:154:LEU:CD2	2.47	0.43
2:H:162:ILE:HD13	2:H:165:LEU:HD12	2.01	0.43
3:I:231:LEU:O	3:I:235:ILE:HG12	2.18	0.43
3:I:80:ARG:O	3:I:83:HIS:HB3	2.19	0.43
1:J:290:GLU:HG2	1:J:342:GLN:HB2	2.00	0.43
1:J:301:GLN:NE2	1:J:359:SER:O	2.51	0.43
1:J:660:LYS:HD3	1:J:660:LYS:HA	1.65	0.43
1:J:686:TYR:O	1:J:691:VAL:HG11	2.19	0.43
2:K:153:LYS:HE2	2:K:153:LYS:HB3	1.77	0.43
2:N:109:GLN:OE1	2:N:137:TRP:NE1	2.43	0.43
3:O:171:ARG:HD3	1:P:724:LEU:HD11	2.00	0.43
1:A:452:THR:HG21	1:A:508:ILE:HG22	2.00	0.43
2:B:152:LEU:HD12	2:B:154:LEU:HD11	2.00	0.43
2:B:313:THR:O	2:B:317:MET:HB2	2.18	0.43
1:D:394:VAL:HG21	3:F:143:THR:HG22	2.00	0.43
1:D:762:ARG:HE	1:D:762:ARG:HA	1.83	0.43
2:E:140:ILE:HG22	2:E:236:MET:HG2	2.01	0.43
3:F:138:PHE:CE1	3:F:140:ILE:HD11	2.54	0.43
3:F:171:ARG:HD3	1:G:724:LEU:HD11	2.01	0.43
1:G:641:TRP:CE3	1:G:750:PRO:HD3	2.53	0.43
2:H:234:CYS:SG	2:H:284:LEU:HB3	2.59	0.43
1:J:301:GLN:CD	1:J:360:TRP:HA	2.39	0.43
1:J:408:ILE:HG23	1:J:414:ILE:N	2.34	0.43
2:K:419:LEU:HD13	2:K:419:LEU:H	1.84	0.43
2:K:495:LYS:HE2	2:K:499:LYS:NZ	2.34	0.43
1:M:218:VAL:HG23	1:M:228:ASN:ND2	2.34	0.43
1:M:274:ILE:HD13	1:M:286:VAL:HB	2.01	0.43
2:N:252:LEU:O	2:N:256:LEU:HB2	2.19	0.43
1:P:301:GLN:CD	1:P:360:TRP:HA	2.38	0.43
1:A:650:LEU:HD22	2:B:242:PHE:HA	2.00	0.43
2:B:329:LYS:O	2:B:332:LEU:N	2.52	0.43
1:A:389:TRP:HH2	3:C:147:GLN:HA	1.81	0.43
3:C:80:ARG:O	3:C:83:HIS:HB3	2.19	0.43
1:D:417:THR:OG1	1:D:451:ILE:HB	2.19	0.43
2:E:153:LYS:HB3	2:E:153:LYS:HE2	1.77	0.43
2:E:194:GLN:HG3	3:F:209:ARG:HH11	1.83	0.43
2:K:286:LEU:HD13	2:K:300:ASN:HB3	2.01	0.43
1:M:207:SER:O	1:M:213:VAL:HG22	2.18	0.43
1:M:301:GLN:CD	1:M:360:TRP:HA	2.39	0.43
1:M:656:HIS:CE1	2:N:171:HIS:HE1	2.37	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:660:LYS:HA	1:M:660:LYS:HD3	1.66	0.43
1:M:721:CYS:HB3	2:N:446:TYR:CD2	2.54	0.43
3:O:15:GLN:HG3	3:O:184:ASN:HD22	1.84	0.43
3:O:361:ASP:HB3	3:O:364:VAL:CG1	2.47	0.43
1:P:323:ASN:N	1:P:323:ASN:OD1	2.50	0.43
2:Q:314:ILE:O	2:Q:318:LEU:HB2	2.18	0.43
2:Q:381:MET:O	2:Q:385:PHE:HB2	2.19	0.43
3:R:421:LYS:HG3	3:R:422:GLY:N	2.33	0.43
2:B:234:CYS:SG	2:B:284:LEU:HB3	2.59	0.43
2:B:290:THR:HB	2:B:292:GLU:N	2.31	0.43
2:B:301:HIS:ND1	2:B:304:LEU:HD12	2.34	0.43
2:B:314:ILE:O	2:B:318:LEU:HB2	2.18	0.43
3:F:435:LEU:O	3:F:439:GLU:HG3	2.19	0.43
1:G:417:THR:OG1	1:G:451:ILE:HB	2.19	0.43
2:H:109:GLN:CD	2:H:137:TRP:HE1	2.21	0.43
2:H:108:PHE:CE1	2:H:156:LEU:HB3	2.54	0.43
2:H:318:LEU:HA	2:H:318:LEU:HD12	1.80	0.43
1:J:362:ARG:NH2	1:J:364:GLU:HG3	2.33	0.43
1:J:63:SER:O	1:J:548:TYR:HD2	2.02	0.43
3:L:410:TYR:O	3:L:413:THR:OG1	2.26	0.43
2:N:290:THR:HB	2:N:292:GLU:N	2.32	0.43
1:P:362:ARG:NH2	1:P:364:GLU:HG3	2.34	0.43
1:P:739:ASP:OD1	2:Q:250:GLN:NE2	2.52	0.43
2:Q:134:LYS:HD3	2:Q:134:LYS:HA	1.79	0.43
2:Q:255:LYS:O	2:Q:259:GLN:HB2	2.18	0.43
1:P:390:GLN:HB2	3:R:151:PRO:O	2.19	0.43
3:R:80:ARG:O	3:R:83:HIS:HB3	2.19	0.43
1:A:301:GLN:CD	1:A:360:TRP:HA	2.39	0.42
1:A:377:ARG:H	1:A:377:ARG:HG3	1.58	0.42
1:A:453:VAL:HA	1:A:465:VAL:O	2.19	0.42
1:A:532:GLU:HB2	1:A:554:ASN:CB	2.49	0.42
1:A:656:HIS:CD2	1:A:656:HIS:N	2.83	0.42
1:A:697:GLU:HG2	1:A:698:LYS:H	1.83	0.42
2:B:255:LYS:O	2:B:259:GLN:HB2	2.19	0.42
1:D:274:ILE:HD13	1:D:286:VAL:HB	2.00	0.42
1:D:675:PHE:HZ	1:D:742:TRP:HZ3	1.66	0.42
3:F:1:MET:HG3	3:F:2:PHE:CD1	2.54	0.42
1:G:344:ILE:HG22	1:G:345:ASP:H	1.84	0.42
1:G:301:GLN:NE2	1:G:359:SER:O	2.52	0.42
1:G:762:ARG:HA	1:G:762:ARG:HE	1.84	0.42
3:I:1:MET:HG3	3:I:2:PHE:CD1	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:381:MET:O	2:K:385:PHE:HB2	2.19	0.42
3:L:27:ILE:HD11	3:L:166:GLU:HA	2.01	0.42
1:M:686:TYR:O	1:M:691:VAL:HG11	2.19	0.42
2:N:178:THR:HG22	2:N:303:GLU:OE1	2.18	0.42
2:N:419:LEU:HD13	2:N:419:LEU:H	1.83	0.42
1:M:389:TRP:HH2	3:O:147:GLN:HA	1.82	0.42
3:O:15:GLN:HA	3:O:18:LYS:HE2	2.01	0.42
3:O:1:MET:HG3	3:O:2:PHE:CD1	2.54	0.42
1:P:443:ASP:O	3:R:3:GLU:N	2.52	0.42
1:P:762:ARG:HA	1:P:762:ARG:HE	1.84	0.42
2:Q:109:GLN:OE1	2:Q:137:TRP:NE1	2.42	0.42
2:Q:495:LYS:HE2	2:Q:499:LYS:NZ	2.34	0.42
2:B:287:TRP:CZ2	2:B:289:ARG:HB3	2.55	0.42
3:C:250:LEU:HB2	3:C:270:PHE:CE2	2.51	0.42
1:D:344:ILE:HG22	1:D:345:ASP:H	1.84	0.42
1:D:363:ILE:O	1:D:363:ILE:HD12	2.19	0.42
3:F:15:GLN:HA	3:F:18:LYS:HE2	2.01	0.42
1:G:532:GLU:HB2	1:G:554:ASN:CB	2.49	0.42
2:H:286:LEU:HD13	2:H:300:ASN:HB3	2.01	0.42
2:H:381:MET:O	2:H:385:PHE:HB2	2.20	0.42
3:I:236:PHE:CZ	3:I:253:ILE:HB	2.54	0.42
3:I:302:ARG:H	3:I:302:ARG:HG2	1.46	0.42
1:J:492:LEU:HD22	1:J:492:LEU:H	1.83	0.42
2:K:109:GLN:CD	2:K:137:TRP:HE1	2.21	0.42
3:L:80:ARG:O	3:L:83:HIS:HB3	2.19	0.42
1:M:227:LEU:HD12	1:M:228:ASN:H	1.84	0.42
1:M:641:TRP:CE3	1:M:750:PRO:HD3	2.54	0.42
1:M:641:TRP:CZ2	1:M:656:HIS:HB3	2.55	0.42
3:O:138:PHE:CE1	3:O:140:ILE:HD11	2.54	0.42
3:O:4:VAL:HG21	3:O:214:VAL:HG22	2.01	0.42
1:P:227:LEU:HD12	1:P:228:ASN:H	1.84	0.42
3:R:291:ARG:HG2	3:R:292:SER:H	1.84	0.42
3:R:4:VAL:HG21	3:R:214:VAL:HG22	2.01	0.42
1:A:362:ARG:NH2	1:A:364:GLU:HG3	2.34	0.42
1:A:637:LEU:HA	1:A:637:LEU:HD22	1.82	0.42
2:B:318:LEU:HA	2:B:318:LEU:HD12	1.81	0.42
2:B:419:LEU:H	2:B:419:LEU:HD13	1.84	0.42
3:C:236:PHE:CE2	3:C:253:ILE:HD12	2.54	0.42
3:C:426:VAL:CG1	3:C:427:PRO:HD3	2.49	0.42
1:D:660:LYS:HA	1:D:660:LYS:HD3	1.65	0.42
2:E:303:GLU:O	2:E:306:VAL:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:250:LEU:HB2	3:F:270:PHE:CE2	2.50	0.42
2:H:329:LYS:O	2:H:332:LEU:N	2.51	0.42
3:I:27:ILE:HD11	3:I:166:GLU:HA	2.01	0.42
3:I:427:PRO:HD3	3:I:430:LEU:HB2	1.99	0.42
1:J:304:ASP:HB2	1:J:363:ILE:O	2.19	0.42
2:K:108:PHE:CE1	2:K:156:LEU:HB3	2.55	0.42
2:K:181:TYR:O	2:K:185:ILE:HG12	2.20	0.42
1:J:394:VAL:HG21	3:L:143:THR:HG22	2.00	0.42
1:A:724:LEU:HD11	3:L:171:ARG:HD3	2.01	0.42
1:M:361:LYS:HA	1:M:375:PHE:O	2.19	0.42
2:N:221:PRO:HD2	2:N:222:PHE:HD2	1.84	0.42
2:N:140:ILE:HG22	2:N:236:MET:HG2	2.01	0.42
2:Q:162:ILE:HD13	2:Q:165:LEU:HD12	2.01	0.42
3:R:236:PHE:CE2	3:R:253:ILE:HD12	2.54	0.42
1:A:304:ASP:HB2	1:A:363:ILE:O	2.19	0.42
1:A:430:ASN:N	1:A:430:ASN:OD1	2.52	0.42
3:C:8:LEU:H	3:C:8:LEU:HD22	1.83	0.42
1:G:390:GLN:HB2	3:I:151:PRO:O	2.18	0.42
2:H:152:LEU:HD13	2:H:152:LEU:HA	1.76	0.42
1:J:192:ASP:OD2	1:J:199:GLY:HA2	2.20	0.42
1:J:290:GLU:OE2	1:J:291:PRO:HD2	2.20	0.42
1:J:361:LYS:HA	1:J:375:PHE:O	2.20	0.42
1:J:532:GLU:HB2	1:J:554:ASN:CB	2.49	0.42
3:L:234:LYS:O	3:L:238:THR:OG1	2.34	0.42
1:M:301:GLN:NE2	1:M:359:SER:O	2.52	0.42
1:M:444:PRO:HG2	1:M:449:LEU:HD11	2.01	0.42
1:M:532:GLU:HB2	1:M:554:ASN:CB	2.49	0.42
2:N:234:CYS:SG	2:N:284:LEU:HB3	2.59	0.42
2:N:255:LYS:O	2:N:259:GLN:HB2	2.18	0.42
3:O:236:PHE:CE2	3:O:253:ILE:HD12	2.54	0.42
2:Q:223:ASN:O	2:Q:497:GLN:NE2	2.52	0.42
3:R:15:GLN:HA	3:R:18:LYS:HE2	2.00	0.42
1:A:413:GLY:HA2	1:A:426:ALA:HB2	2.02	0.42
2:B:152:LEU:HB3	2:B:154:LEU:CD2	2.48	0.42
2:B:129:PHE:HE1	2:B:169:SER:N	2.17	0.42
2:B:366:TYR:HA	2:B:369:TRP:CD1	2.54	0.42
3:C:15:GLN:HA	3:C:18:LYS:HE2	2.00	0.42
1:A:443:ASP:O	3:C:3:GLU:N	2.53	0.42
2:E:408:ILE:HD11	2:E:412:LYS:HE3	2.01	0.42
3:F:318:ILE:O	3:F:321:GLN:HB3	2.20	0.42
3:F:427:PRO:HD3	3:F:430:LEU:HB2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:641:TRP:CZ2	1:G:656:HIS:HB3	2.54	0.42
1:J:632:ILE:O	1:J:636:GLU:HG3	2.19	0.42
2:K:96:ILE:HB	2:K:100:ALA:HB2	2.00	0.42
3:L:308:PHE:HD1	3:L:309:ALA:H	1.67	0.42
1:M:265:THR:OG1	1:M:268:SER:N	2.41	0.42
1:M:290:GLU:HG2	1:M:342:GLN:HB2	2.01	0.42
2:N:162:ILE:HD13	2:N:165:LEU:HD12	2.02	0.42
2:N:386:LEU:HD13	3:O:241:ARG:NH2	2.34	0.42
1:P:290:GLU:HG2	1:P:342:GLN:HB2	2.01	0.42
1:P:363:ILE:HD12	1:P:363:ILE:O	2.19	0.42
1:P:412:ASN:O	1:P:426:ALA:HB1	2.19	0.42
2:Q:258:MET:HB3	2:Q:258:MET:HE2	1.93	0.42
3:R:138:PHE:CE1	3:R:140:ILE:HD11	2.55	0.42
1:A:314:GLN:OE1	1:A:314:GLN:HA	2.19	0.42
1:A:363:ILE:O	1:A:363:ILE:HD12	2.19	0.42
2:B:286:LEU:HD13	2:B:300:ASN:HB3	2.02	0.42
3:C:312:TYR:HA	3:C:315:SER:HG	1.83	0.42
1:D:361:LYS:HA	1:D:375:PHE:O	2.19	0.42
1:D:504:THR:HG23	1:D:505:PRO:HD2	2.02	0.42
2:E:162:ILE:HD13	2:E:165:LEU:HD12	2.02	0.42
1:G:314:GLN:HA	1:G:314:GLN:OE1	2.19	0.42
1:G:720:GLN:O	1:G:723:VAL:HG12	2.19	0.42
2:H:262:LEU:HD23	2:H:262:LEU:HA	1.87	0.42
1:J:265:THR:HG1	1:J:268:SER:H	1.65	0.42
1:J:474:LYS:HA	1:J:505:PRO:HD2	2.02	0.42
2:K:162:ILE:HD13	2:K:165:LEU:HD12	2.01	0.42
2:K:287:TRP:CZ2	2:K:289:ARG:HB3	2.55	0.42
1:J:574:TRP:CH2	2:K:495:LYS:HD2	2.54	0.42
3:L:11:ARG:HG3	3:L:11:ARG:H	1.48	0.42
3:L:15:GLN:HG3	3:L:184:ASN:HD22	1.84	0.42
1:M:417:THR:OG1	1:M:451:ILE:HB	2.19	0.42
1:M:739:ASP:OD1	2:N:250:GLN:NE2	2.52	0.42
2:N:287:TRP:CZ2	2:N:289:ARG:HB3	2.55	0.42
3:O:427:PRO:HB2	3:O:428:SER:H	1.75	0.42
1:P:321:LYS:HD3	1:P:321:LYS:N	2.21	0.42
1:P:301:GLN:NE2	1:P:359:SER:O	2.52	0.42
1:P:61:VAL:HB	1:P:551:ALA:HB3	2.01	0.42
1:P:762:ARG:HB3	2:Q:138:LEU:HD13	2.01	0.42
2:Q:234:CYS:SG	2:Q:284:LEU:HB3	2.59	0.42
3:R:24:ILE:O	3:R:28:SER:OG	2.34	0.42
1:A:417:THR:OG1	1:A:451:ILE:HB	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:286:LEU:CD2	2:B:300:ASN:HB3	2.50	0.42
3:C:27:ILE:HD11	3:C:166:GLU:HA	2.02	0.42
1:D:453:VAL:HA	1:D:465:VAL:O	2.19	0.42
2:E:109:GLN:OE1	2:E:137:TRP:NE1	2.42	0.42
1:D:762:ARG:HB3	2:E:138:LEU:HD13	2.02	0.42
2:E:512:ARG:HD3	2:E:512:ARG:HA	1.83	0.42
3:F:236:PHE:CZ	3:F:253:ILE:HB	2.55	0.42
1:G:192:ASP:OD2	1:G:199:GLY:HA2	2.20	0.42
1:G:611:ILE:CD1	1:G:731:LEU:HB2	2.50	0.42
1:J:453:VAL:HA	1:J:465:VAL:O	2.20	0.42
1:J:720:GLN:O	1:J:723:VAL:HG12	2.19	0.42
2:K:341:ARG:HD3	2:K:373:GLU:OE2	2.19	0.42
3:L:236:PHE:CE2	3:L:253:ILE:HD12	2.54	0.42
1:M:377:ARG:NH2	1:M:378:SER:OG	2.34	0.42
1:M:412:ASN:O	1:M:426:ALA:HB1	2.20	0.42
1:M:413:GLY:HA2	1:M:426:ALA:HB2	2.02	0.42
1:M:762:ARG:HG3	2:N:139:LYS:NZ	2.35	0.42
2:N:286:LEU:HD13	2:N:300:ASN:HB3	2.02	0.42
2:N:374:THR:O	2:N:377:PHE:HB3	2.20	0.42
1:M:390:GLN:HB2	3:O:151:PRO:O	2.20	0.42
3:O:235:ILE:H	3:O:235:ILE:HG12	1.61	0.42
1:P:408:ILE:HG23	1:P:414:ILE:N	2.35	0.42
2:Q:286:LEU:HD13	2:Q:300:ASN:HB3	2.01	0.42
1:P:389:TRP:HH2	3:R:147:GLN:HA	1.83	0.42
3:R:1:MET:HG3	3:R:2:PHE:CD1	2.54	0.42
3:R:318:ILE:O	3:R:321:GLN:HB3	2.20	0.42
1:A:290:GLU:HG2	1:A:342:GLN:HB2	2.02	0.42
1:A:444:PRO:HG2	1:A:449:LEU:HD11	2.01	0.42
1:A:61:VAL:HB	1:A:551:ALA:HB3	2.02	0.42
1:A:721:CYS:HB3	2:B:446:TYR:CD2	2.54	0.42
2:B:153:LYS:HB3	2:B:153:LYS:HE2	1.77	0.42
1:D:290:GLU:HG2	1:D:342:GLN:HB2	2.01	0.42
2:E:159:THR:O	2:E:163:SER:HB2	2.20	0.42
2:E:234:CYS:SG	2:E:284:LEU:HB3	2.59	0.42
1:G:433:VAL:HG22	1:G:434:ARG:O	2.20	0.42
1:G:660:LYS:HD3	1:G:660:LYS:HA	1.65	0.42
1:G:728:GLN:HB3	1:G:731:LEU:HB3	2.01	0.42
3:I:15:GLN:HB2	3:I:15:GLN:HE21	1.66	0.42
1:J:344:ILE:HG22	1:J:345:ASP:H	1.85	0.42
1:J:430:ASN:OD1	1:J:430:ASN:N	2.53	0.42
3:L:138:PHE:CE1	3:L:140:ILE:HD11	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:150:GLN:H	3:L:150:GLN:HG2	1.35	0.42
3:L:426:VAL:CG1	3:L:427:PRO:HD3	2.49	0.42
3:L:435:LEU:O	3:L:439:GLU:HG3	2.19	0.42
1:M:690:ASP:OD1	1:M:750:PRO:HB3	2.19	0.42
3:O:8:LEU:HD22	3:O:8:LEU:H	1.84	0.42
1:P:686:TYR:O	1:P:691:VAL:HG11	2.19	0.42
2:Q:140:ILE:HG22	2:Q:236:MET:HG2	2.01	0.42
3:R:236:PHE:CZ	3:R:253:ILE:HB	2.55	0.42
3:R:427:PRO:HB2	3:R:428:SER:H	1.75	0.42
1:A:185:GLN:HG3	1:A:186:TYR:N	2.35	0.42
1:A:227:LEU:HD12	1:A:228:ASN:H	1.84	0.42
1:A:301:GLN:NE2	1:A:359:SER:O	2.52	0.42
3:C:138:PHE:CE1	3:C:140:ILE:HD11	2.54	0.42
3:C:15:GLN:HG3	3:C:184:ASN:HD22	1.85	0.42
3:C:314:TRP:CD1	3:C:367:ILE:HD11	2.55	0.42
1:D:185:GLN:HG3	1:D:186:TYR:H	1.84	0.42
1:D:192:ASP:OD2	1:D:199:GLY:HA2	2.20	0.42
1:D:301:GLN:NE2	1:D:359:SER:O	2.53	0.42
1:D:690:ASP:OD1	1:D:750:PRO:HB3	2.18	0.42
2:E:366:TYR:HA	2:E:369:TRP:CD1	2.55	0.42
2:E:410:ARG:HA	2:E:413:LEU:CB	2.45	0.42
3:F:25:ASN:O	3:F:29:ARG:HB2	2.20	0.42
1:G:377:ARG:H	1:G:377:ARG:HG3	1.57	0.42
3:I:250:LEU:HB2	3:I:270:PHE:CE2	2.51	0.42
1:J:363:ILE:HD12	1:J:363:ILE:O	2.19	0.42
1:J:433:VAL:HG22	1:J:434:ARG:O	2.20	0.42
1:J:641:TRP:CE3	1:J:750:PRO:HD3	2.54	0.42
2:K:152:LEU:HB3	2:K:154:LEU:CD2	2.48	0.42
3:L:236:PHE:CZ	3:L:253:ILE:HB	2.55	0.42
3:L:8:LEU:HD22	3:L:8:LEU:H	1.84	0.42
2:N:262:LEU:HD23	2:N:262:LEU:HA	1.86	0.42
3:O:247:ILE:HG12	3:O:247:ILE:H	1.62	0.42
1:P:417:THR:OG1	1:P:451:ILE:HB	2.19	0.42
2:Q:252:LEU:O	2:Q:256:LEU:HB2	2.19	0.42
3:R:426:VAL:CG1	3:R:427:PRO:HD3	2.48	0.42
1:A:584:ARG:O	1:A:588:SER:CB	2.66	0.42
1:A:63:SER:O	1:A:548:TYR:HD2	2.03	0.42
2:B:109:GLN:CD	2:B:137:TRP:HE1	2.21	0.42
2:B:162:ILE:HD13	2:B:165:LEU:HD12	2.02	0.42
2:B:310:PHE:O	2:B:314:ILE:HG13	2.20	0.42
3:C:435:LEU:O	3:C:439:GLU:HG3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:218:VAL:HG23	1:D:228:ASN:ND2	2.34	0.42
1:D:329:ILE:HG13	1:D:330:PRO:N	2.33	0.42
1:G:362:ARG:NH2	1:G:364:GLU:HG3	2.34	0.42
2:H:181:TYR:O	2:H:185:ILE:HG12	2.20	0.42
2:H:439:ILE:H	2:H:439:ILE:HG13	1.65	0.42
3:I:138:PHE:CE1	3:I:140:ILE:HD11	2.55	0.42
3:I:168:ILE:HD11	3:I:172:LYS:HE2	2.02	0.42
3:I:318:ILE:O	3:I:321:GLN:HB3	2.20	0.42
1:J:314:GLN:HA	1:J:314:GLN:OE1	2.19	0.42
3:L:25:ASN:O	3:L:29:ARG:HB2	2.20	0.42
1:M:304:ASP:HB2	1:M:363:ILE:O	2.20	0.42
1:M:408:ILE:HG23	1:M:414:ILE:N	2.35	0.42
2:N:108:PHE:CE1	2:N:156:LEU:HB3	2.54	0.42
3:O:273:TRP:CZ3	3:O:274:MET:HG2	2.55	0.42
3:O:435:LEU:O	3:O:439:GLU:HG3	2.20	0.42
1:P:304:ASP:HB2	1:P:363:ILE:O	2.20	0.42
1:P:720:GLN:O	1:P:723:VAL:HG12	2.20	0.42
2:Q:160:SER:HA	2:Q:163:SER:HB2	2.02	0.42
2:Q:413:LEU:HA	2:Q:416:ILE:HD12	2.02	0.42
1:A:185:GLN:HG3	1:A:186:TYR:H	1.84	0.41
1:A:347:LEU:H	1:A:347:LEU:HD12	1.85	0.41
3:C:318:ILE:O	3:C:321:GLN:HB3	2.20	0.41
1:D:227:LEU:HD12	1:D:228:ASN:H	1.84	0.41
1:D:456:VAL:HB	1:D:463:LEU:CD2	2.50	0.41
2:E:108:PHE:CE1	2:E:156:LEU:HB3	2.54	0.41
2:E:286:LEU:HD13	2:E:300:ASN:HB3	2.02	0.41
3:F:171:ARG:C	3:F:174:GLU:H	2.21	0.41
1:G:762:ARG:HG3	2:H:139:LYS:NZ	2.35	0.41
3:I:25:ASN:O	3:I:29:ARG:HB2	2.20	0.41
1:J:274:ILE:HD13	1:J:286:VAL:HB	2.00	0.41
3:L:4:VAL:HG21	3:L:214:VAL:HG22	2.02	0.41
3:L:273:TRP:CZ3	3:L:274:MET:HG2	2.55	0.41
1:M:443:ASP:O	3:O:3:GLU:N	2.53	0.41
1:P:480:VAL:HB	1:P:492:LEU:CD2	2.44	0.41
2:Q:318:LEU:HA	2:Q:318:LEU:HD12	1.81	0.41
2:Q:194:GLN:HG3	3:R:209:ARG:HH11	1.85	0.41
1:A:408:ILE:HG23	1:A:414:ILE:N	2.35	0.41
1:A:574:TRP:HB3	1:A:578:PHE:CE2	2.55	0.41
3:C:173:MET:O	3:C:176:PRO:HD2	2.20	0.41
1:D:185:GLN:HG3	1:D:186:TYR:N	2.35	0.41
1:D:394:VAL:HG22	1:D:434:ARG:NH1	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:412:ASN:O	1:D:426:ALA:HB1	2.20	0.41
1:D:433:VAL:HG22	1:D:434:ARG:O	2.20	0.41
1:D:641:TRP:CE3	1:D:750:PRO:HD3	2.55	0.41
1:D:721:CYS:HB3	2:E:446:TYR:CD2	2.55	0.41
3:F:15:GLN:HG3	3:F:184:ASN:HD22	1.84	0.41
1:G:596:ILE:O	1:G:596:ILE:HD12	2.20	0.41
2:H:341:ARG:HD3	2:H:373:GLU:OE2	2.20	0.41
2:H:366:TYR:HA	2:H:369:TRP:CD1	2.54	0.41
3:I:171:ARG:HD3	1:J:724:LEU:HD11	2.03	0.41
2:K:223:ASN:O	2:K:497:GLN:NE2	2.53	0.41
2:K:329:LYS:O	2:K:332:LEU:N	2.53	0.41
1:M:320:ILE:O	1:M:322:GLY:N	2.53	0.41
3:C:171:ARG:HD3	1:M:724:LEU:HD11	2.02	0.41
2:N:159:THR:O	2:N:163:SER:HB2	2.20	0.41
2:N:160:SER:HA	2:N:163:SER:HB2	2.02	0.41
3:O:365:TRP:HB3	3:O:418:CYS:HB2	2.02	0.41
1:P:185:GLN:HG3	1:P:186:TYR:N	2.35	0.41
1:P:314:GLN:HA	1:P:314:GLN:OE1	2.20	0.41
1:P:430:ASN:OD1	1:P:430:ASN:N	2.52	0.41
1:P:656:HIS:CD2	1:P:656:HIS:N	2.84	0.41
2:Q:313:THR:O	2:Q:317:MET:HB2	2.21	0.41
2:Q:329:LYS:O	2:Q:332:LEU:N	2.53	0.41
2:Q:334:LEU:HD12	2:Q:334:LEU:HA	1.90	0.41
3:R:361:ASP:HB3	3:R:364:VAL:CG1	2.48	0.41
1:A:762:ARG:HG3	2:B:139:LYS:NZ	2.35	0.41
3:C:165:ILE:HG13	3:C:165:ILE:H	1.67	0.41
1:D:413:GLY:HA2	1:D:426:ALA:HB2	2.02	0.41
1:D:686:TYR:O	1:D:691:VAL:HG11	2.20	0.41
2:E:109:GLN:CD	2:E:137:TRP:HE1	2.21	0.41
2:E:318:LEU:HA	2:E:318:LEU:HD12	1.81	0.41
2:E:413:LEU:HA	2:E:416:ILE:HD12	2.02	0.41
3:F:361:ASP:HB3	3:F:364:VAL:CG1	2.48	0.41
1:G:329:ILE:HG13	1:G:330:PRO:N	2.33	0.41
1:G:290:GLU:HG2	1:G:342:GLN:HB2	2.01	0.41
2:H:194:GLN:HG3	3:I:209:ARG:NH1	2.35	0.41
2:H:226:LEU:O	2:H:230:ILE:HG23	2.20	0.41
3:I:24:ILE:HA	3:I:24:ILE:HD13	1.95	0.41
3:I:426:VAL:CG1	3:I:427:PRO:HD3	2.50	0.41
1:J:551:ALA:O	1:J:552:LEU:HD23	2.21	0.41
2:K:160:SER:HA	2:K:163:SER:HB2	2.02	0.41
2:K:356:VAL:HG11	3:L:208:TYR:CD1	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:1:MET:HG3	3:L:2:PHE:CD1	2.55	0.41
1:M:290:GLU:OE2	1:M:291:PRO:HD2	2.20	0.41
1:M:56:ASP:O	1:M:57:LEU:HD13	2.20	0.41
3:O:426:VAL:CG1	3:O:427:PRO:HD3	2.49	0.41
1:P:444:PRO:HG2	1:P:449:LEU:HD11	2.03	0.41
1:P:574:TRP:CH2	2:Q:495:LYS:HD2	2.54	0.41
1:A:408:ILE:HG23	1:A:413:GLY:C	2.40	0.41
2:B:435:GLN:HG3	2:B:435:GLN:H	1.42	0.41
1:A:574:TRP:CH2	2:B:495:LYS:HD2	2.55	0.41
1:A:390:GLN:HB2	3:C:151:PRO:O	2.20	0.41
2:B:386:LEU:HD13	3:C:241:ARG:NH2	2.34	0.41
3:C:273:TRP:CZ3	3:C:274:MET:HG2	2.56	0.41
3:C:361:ASP:HB3	3:C:364:VAL:CG1	2.48	0.41
1:G:248:PRO:HB3	1:G:305:PHE:HB2	2.03	0.41
1:G:274:ILE:HD13	1:G:286:VAL:HB	2.01	0.41
3:I:435:LEU:O	3:I:439:GLU:HG3	2.20	0.41
1:J:413:GLY:HA2	1:J:426:ALA:HB2	2.01	0.41
1:M:632:ILE:O	1:M:636:GLU:HG3	2.19	0.41
2:N:120:ILE:HA	2:N:125:PHE:HB2	2.03	0.41
2:N:329:LYS:O	2:N:332:LEU:N	2.53	0.41
3:O:275:CYS:O	3:O:279:SER:HB3	2.21	0.41
3:O:314:TRP:CD1	3:O:367:ILE:HD11	2.55	0.41
3:O:34:ILE:HD12	3:O:34:ILE:HA	1.89	0.41
3:O:80:ARG:O	3:O:83:HIS:HB3	2.19	0.41
1:P:185:GLN:HG3	1:P:186:TYR:H	1.85	0.41
1:P:454:GLN:HB3	1:P:465:VAL:HG23	2.02	0.41
1:P:484:ARG:HB2	1:P:488:LEU:HB3	2.01	0.41
1:P:63:SER:O	1:P:548:TYR:HD2	2.03	0.41
1:P:641:TRP:CE3	1:P:750:PRO:HD3	2.55	0.41
3:R:171:ARG:C	3:R:174:GLU:H	2.20	0.41
3:R:25:ASN:O	3:R:29:ARG:HB2	2.20	0.41
1:A:192:ASP:OD2	1:A:199:GLY:HA2	2.19	0.41
2:B:120:ILE:HA	2:B:125:PHE:HB2	2.03	0.41
1:D:248:PRO:HB3	1:D:305:PHE:HB2	2.02	0.41
1:D:390:GLN:HB2	3:F:151:PRO:O	2.20	0.41
1:D:641:TRP:CZ2	1:D:656:HIS:HB3	2.55	0.41
1:D:762:ARG:HG3	2:E:139:LYS:NZ	2.35	0.41
1:G:430:ASN:OD1	1:G:430:ASN:N	2.53	0.41
1:G:484:ARG:HB2	1:G:488:LEU:HB3	2.02	0.41
1:J:412:ASN:O	1:J:426:ALA:HB1	2.20	0.41
2:K:226:LEU:O	2:K:230:ILE:HG23	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:194:GLN:HG3	3:L:209:ARG:HH11	1.85	0.41
3:L:304:HIS:CD2	3:L:306:ALA:HA	2.56	0.41
3:L:318:ILE:O	3:L:321:GLN:HB3	2.20	0.41
1:M:248:PRO:HB3	1:M:305:PHE:HB2	2.03	0.41
1:M:344:ILE:HG22	1:M:345:ASP:H	1.84	0.41
1:M:484:ARG:HB2	1:M:488:LEU:HB3	2.01	0.41
1:M:762:ARG:HB3	2:N:138:LEU:HD13	2.02	0.41
2:N:194:GLN:HG3	3:O:209:ARG:HH11	1.85	0.41
1:P:394:VAL:HG22	1:P:434:ARG:NH1	2.36	0.41
1:P:413:GLY:HA2	1:P:426:ALA:HB2	2.01	0.41
1:P:504:THR:HG23	1:P:505:PRO:HD2	2.03	0.41
2:Q:410:ARG:HA	2:Q:413:LEU:CB	2.45	0.41
1:A:290:GLU:OE2	1:A:291:PRO:HD2	2.21	0.41
1:A:248:PRO:HB3	1:A:305:PHE:HB2	2.03	0.41
1:A:474:LYS:HA	1:A:505:PRO:HD2	2.03	0.41
1:A:686:TYR:O	1:A:691:VAL:HG11	2.20	0.41
2:B:303:GLU:O	2:B:306:VAL:N	2.53	0.41
2:B:194:GLN:HG3	3:C:209:ARG:NH1	2.34	0.41
3:C:4:VAL:HG21	3:C:214:VAL:HG22	2.02	0.41
1:D:420:GLU:HA	1:D:442:LEU:H	1.86	0.41
1:D:551:ALA:O	1:D:552:LEU:HD23	2.20	0.41
1:D:720:GLN:O	1:D:723:VAL:HG12	2.20	0.41
2:E:287:TRP:CZ2	2:E:289:ARG:HB3	2.55	0.41
3:F:273:TRP:CZ3	3:F:274:MET:HG2	2.55	0.41
2:H:310:PHE:O	2:H:314:ILE:HG13	2.19	0.41
3:I:273:TRP:CZ3	3:I:274:MET:HG2	2.55	0.41
3:I:417:ILE:HA	3:I:417:ILE:HD12	1.98	0.41
1:J:227:LEU:HD12	1:J:228:ASN:H	1.84	0.41
1:J:248:PRO:HB3	1:J:305:PHE:HB2	2.03	0.41
1:J:329:ILE:HG13	1:J:330:PRO:N	2.33	0.41
1:J:56:ASP:O	1:J:57:LEU:HD13	2.21	0.41
1:J:574:TRP:HB3	1:J:578:PHE:CE2	2.56	0.41
2:K:313:THR:O	2:K:317:MET:HB2	2.20	0.41
1:M:314:GLN:HA	1:M:314:GLN:OE1	2.19	0.41
1:M:352:PHE:CE1	3:O:157:MET:HG2	2.56	0.41
1:M:363:ILE:O	1:M:363:ILE:HD12	2.20	0.41
1:M:453:VAL:HA	1:M:465:VAL:O	2.20	0.41
1:M:599:LYS:HG2	2:N:272:GLN:NE2	2.36	0.41
3:O:236:PHE:CZ	3:O:253:ILE:HB	2.56	0.41
3:O:318:ILE:O	3:O:321:GLN:HB3	2.19	0.41
1:P:408:ILE:HG23	1:P:413:GLY:C	2.40	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:R:152:ILE:HG13	3:R:153:ASN:N	2.36	0.41
3:R:314:TRP:CD1	3:R:367:ILE:HD11	2.56	0.41
1:A:329:ILE:HG13	1:A:330:PRO:N	2.33	0.41
1:D:430:ASN:OD1	1:D:430:ASN:N	2.53	0.41
1:D:762:ARG:HA	1:D:762:ARG:NE	2.35	0.41
2:E:223:ASN:O	2:E:497:GLN:NE2	2.53	0.41
3:F:152:ILE:HG13	3:F:153:ASN:N	2.36	0.41
3:F:15:GLN:HB2	3:F:15:GLN:HE21	1.64	0.41
3:F:421:LYS:HG3	3:F:422:GLY:N	2.32	0.41
3:F:427:PRO:HB2	3:F:428:SER:H	1.75	0.41
3:F:4:VAL:HG21	3:F:214:VAL:HG22	2.02	0.41
1:G:227:LEU:HD12	1:G:228:ASN:H	1.84	0.41
1:G:468:VAL:HG13	1:G:477:TYR:O	2.21	0.41
1:G:504:THR:HG23	1:G:505:PRO:HD2	2.02	0.41
1:J:468:VAL:HG13	1:J:477:TYR:O	2.20	0.41
1:J:484:ARG:HB2	1:J:488:LEU:HB3	2.02	0.41
1:J:762:ARG:NE	1:J:762:ARG:HA	2.35	0.41
2:K:301:HIS:ND1	2:K:304:LEU:HD12	2.35	0.41
1:M:504:THR:HG23	1:M:505:PRO:HD2	2.03	0.41
2:N:128:GLU:O	2:N:132:VAL:HG23	2.20	0.41
3:O:152:ILE:HG13	3:O:153:ASN:N	2.36	0.41
3:O:15:GLN:HB2	3:O:15:GLN:HE21	1.66	0.41
1:P:453:VAL:HA	1:P:465:VAL:O	2.21	0.41
1:P:584:ARG:O	1:P:588:SER:CB	2.66	0.41
1:P:762:ARG:HG3	2:Q:139:LYS:NZ	2.36	0.41
1:A:412:ASN:O	1:A:426:ALA:HB1	2.21	0.41
1:A:468:VAL:HG13	1:A:477:TYR:O	2.21	0.41
1:A:56:ASP:O	1:A:57:LEU:HD13	2.20	0.41
2:B:283:ASN:O	2:B:284:LEU:HD12	2.21	0.41
2:B:410:ARG:HE	2:B:413:LEU:HD13	1.86	0.41
3:C:34:ILE:HD12	3:C:34:ILE:HA	1.89	0.41
3:C:427:PRO:HB2	3:C:428:SER:H	1.75	0.41
1:D:362:ARG:NH2	1:D:364:GLU:HG3	2.35	0.41
1:D:596:ILE:O	1:D:596:ILE:HD12	2.21	0.41
2:E:152:LEU:HD13	2:E:152:LEU:HA	1.77	0.41
3:F:314:TRP:CD1	3:F:367:ILE:HD11	2.56	0.41
1:G:453:VAL:HA	1:G:465:VAL:O	2.20	0.41
1:G:686:TYR:O	1:G:691:VAL:HG11	2.20	0.41
1:G:656:HIS:HE1	2:H:171:HIS:CE1	2.39	0.41
2:H:221:PRO:HD2	2:H:222:PHE:HD2	1.85	0.41
3:I:15:GLN:HG3	3:I:184:ASN:HD22	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:421:ILE:HA	1:J:440:HIS:O	2.21	0.41
2:K:120:ILE:HA	2:K:125:PHE:HB2	2.03	0.41
2:K:128:GLU:O	2:K:132:VAL:HG23	2.21	0.41
2:K:286:LEU:CD2	2:K:300:ASN:HB3	2.50	0.41
3:L:152:ILE:HG13	3:L:153:ASN:N	2.36	0.41
1:M:185:GLN:HG3	1:M:186:TYR:N	2.36	0.41
1:M:185:GLN:HG3	1:M:186:TYR:H	1.86	0.41
1:M:433:VAL:HG22	1:M:434:ARG:O	2.20	0.41
1:M:468:VAL:HG13	1:M:477:TYR:O	2.21	0.41
3:O:304:HIS:CD2	3:O:306:ALA:HA	2.55	0.41
1:P:248:PRO:HB3	1:P:305:PHE:HB2	2.03	0.41
1:P:456:VAL:HB	1:P:463:LEU:CD2	2.51	0.41
1:P:728:GLN:HB3	1:P:731:LEU:HB3	2.02	0.41
3:R:34:ILE:HD12	3:R:34:ILE:HA	1.89	0.41
1:A:444:PRO:CG	1:A:449:LEU:HD11	2.51	0.41
1:A:768:TYR:O	1:A:771:ILE:HB	2.21	0.41
2:B:160:SER:HA	2:B:163:SER:HB2	2.03	0.41
2:B:374:THR:HG23	3:C:219:LEU:HD13	2.02	0.41
3:F:312:TYR:HA	3:F:315:SER:HG	1.85	0.41
3:F:365:TRP:HB3	3:F:418:CYS:HB2	2.02	0.41
1:G:304:ASP:HB2	1:G:363:ILE:O	2.21	0.41
1:G:456:VAL:HB	1:G:463:LEU:CD2	2.51	0.41
1:G:63:SER:O	1:G:548:TYR:HD2	2.03	0.41
2:H:287:TRP:CZ2	2:H:289:ARG:HB3	2.55	0.41
2:H:303:GLU:O	2:H:306:VAL:N	2.54	0.41
3:I:200:THR:O	3:I:204:GLU:HG2	2.21	0.41
3:I:275:CYS:O	3:I:279:SER:HB3	2.21	0.41
3:I:365:TRP:HB3	3:I:418:CYS:HB2	2.03	0.41
1:J:596:ILE:O	1:J:596:ILE:HD12	2.20	0.41
2:K:194:GLN:HG3	3:L:209:ARG:NH1	2.35	0.41
2:K:221:PRO:HD2	2:K:222:PHE:HD2	1.86	0.41
2:K:413:LEU:HA	2:K:416:ILE:HD12	2.02	0.41
2:N:194:GLN:HG3	3:O:209:ARG:NH1	2.36	0.41
1:P:596:ILE:HD12	1:P:596:ILE:O	2.20	0.41
1:P:762:ARG:HA	1:P:762:ARG:NE	2.36	0.41
2:Q:247:ILE:HD12	2:Q:247:ILE:HA	1.89	0.41
3:R:275:CYS:O	3:R:279:SER:HB3	2.21	0.41
1:A:377:ARG:NH2	1:A:378:SER:OG	2.34	0.41
1:A:433:VAL:HG22	1:A:434:ARG:O	2.21	0.41
1:A:504:THR:HG23	1:A:505:PRO:HD2	2.02	0.41
1:A:762:ARG:NE	1:A:762:ARG:HA	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:221:PRO:HD2	2:B:222:PHE:HD2	1.86	0.41
2:B:352:ILE:HD12	2:B:380:TRP:CE3	2.56	0.41
2:B:412:LYS:O	2:B:416:ILE:HG13	2.21	0.41
2:B:512:ARG:HD3	2:B:512:ARG:HA	1.83	0.41
3:C:200:THR:O	3:C:204:GLU:HG2	2.21	0.41
3:C:275:CYS:O	3:C:279:SER:HB3	2.21	0.41
2:E:332:LEU:HD13	2:E:332:LEU:HA	1.78	0.41
3:F:219:LEU:HA	3:F:219:LEU:HD23	1.83	0.41
3:F:305:THR:HB	3:F:308:PHE:CE1	2.56	0.41
3:F:364:VAL:HA	3:F:367:ILE:HB	2.03	0.41
3:F:426:VAL:CG1	3:F:427:PRO:HD3	2.49	0.41
1:G:408:ILE:HG23	1:G:414:ILE:N	2.36	0.41
1:G:584:ARG:O	1:G:588:SER:CB	2.67	0.41
2:H:160:SER:HA	2:H:163:SER:HB2	2.02	0.41
2:H:255:LYS:O	2:H:259:GLN:HB2	2.20	0.41
2:H:410:ARG:HE	2:H:413:LEU:HD13	1.86	0.41
3:I:410:TYR:O	3:I:413:THR:OG1	2.26	0.41
1:J:456:VAL:HB	1:J:463:LEU:CD2	2.51	0.41
2:K:439:ILE:HG13	2:K:439:ILE:H	1.64	0.41
1:M:192:ASP:OD2	1:M:199:GLY:HA2	2.20	0.41
1:M:408:ILE:HG23	1:M:413:GLY:C	2.41	0.41
1:M:474:LYS:HA	1:M:505:PRO:HD2	2.02	0.41
1:M:63:SER:O	1:M:548:TYR:HD2	2.03	0.41
1:M:596:ILE:HD12	1:M:596:ILE:O	2.20	0.41
1:M:611:ILE:HD11	1:M:731:LEU:HB2	2.03	0.41
1:P:344:ILE:HG22	1:P:345:ASP:H	1.86	0.41
1:P:641:TRP:CZ2	1:P:656:HIS:HB3	2.56	0.41
2:Q:120:ILE:HA	2:Q:125:PHE:HB2	2.03	0.41
2:Q:287:TRP:CZ2	2:Q:289:ARG:HB3	2.55	0.41
3:R:247:ILE:HG12	3:R:247:ILE:H	1.62	0.41
3:R:312:TYR:HA	3:R:315:SER:HG	1.85	0.41
1:A:596:ILE:O	1:A:596:ILE:HD12	2.20	0.41
3:C:15:GLN:HB2	3:C:15:GLN:HE21	1.65	0.41
1:D:384:ASP:CB	1:D:389:TRP:HB3	2.46	0.41
1:D:454:GLN:HB3	1:D:465:VAL:HG23	2.03	0.41
1:D:484:ARG:HB2	1:D:488:LEU:HB3	2.02	0.41
1:D:728:GLN:HB3	1:D:731:LEU:HB3	2.02	0.41
1:D:574:TRP:CH2	2:E:495:LYS:HD2	2.56	0.41
3:F:8:LEU:H	3:F:8:LEU:HD22	1.85	0.41
1:G:185:GLN:HG3	1:G:186:TYR:N	2.36	0.41
1:G:444:PRO:HG2	1:G:449:LEU:HD11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:161:ASN:O	3:I:165:ILE:HG13	2.21	0.41
1:J:377:ARG:NH2	1:J:378:SER:OG	2.35	0.41
2:K:104:PHE:CD2	2:K:105:LEU:HD23	2.56	0.41
2:K:290:THR:HB	2:K:292:GLU:N	2.32	0.41
3:L:168:ILE:HD11	3:L:172:LYS:HE2	2.03	0.41
1:M:454:GLN:HB3	1:M:465:VAL:HG23	2.02	0.41
1:P:468:VAL:HG13	1:P:477:TYR:O	2.21	0.41
1:P:574:TRP:HB3	1:P:578:PHE:CE2	2.55	0.41
1:P:675:PHE:HZ	1:P:742:TRP:CZ3	2.39	0.41
2:Q:194:GLN:HG3	3:R:209:ARG:NH1	2.36	0.41
2:Q:286:LEU:CD2	2:Q:300:ASN:HB3	2.49	0.41
3:R:15:GLN:HB2	3:R:15:GLN:HE21	1.65	0.41
3:R:364:VAL:HA	3:R:367:ILE:HB	2.03	0.41
1:A:344:ILE:HG22	1:A:345:ASP:H	1.86	0.40
1:A:421:ILE:HA	1:A:440:HIS:O	2.22	0.40
1:A:641:TRP:CE3	1:A:750:PRO:HD3	2.56	0.40
1:D:473:HIS:C	1:D:504:THR:HG23	2.41	0.40
1:D:611:ILE:CD1	1:D:731:LEU:HB2	2.51	0.40
2:E:410:ARG:HE	2:E:413:LEU:HD13	1.86	0.40
1:G:320:ILE:O	1:G:322:GLY:N	2.54	0.40
1:G:768:TYR:O	1:G:771:ILE:HB	2.21	0.40
2:H:193:PHE:CE2	3:I:208:TYR:CD1	3.10	0.40
3:I:23:TYR:CZ	3:I:27:ILE:HG13	2.56	0.40
3:I:314:TRP:CD1	3:I:367:ILE:HD11	2.55	0.40
1:J:611:ILE:CD1	1:J:731:LEU:HB2	2.51	0.40
2:K:386:LEU:HD13	3:L:241:ARG:NH2	2.36	0.40
1:M:430:ASN:N	1:M:430:ASN:OD1	2.53	0.40
1:M:456:VAL:HB	1:M:463:LEU:CD2	2.51	0.40
2:N:134:LYS:HA	2:N:134:LYS:HD3	1.79	0.40
2:N:153:LYS:HE2	2:N:153:LYS:HB3	1.77	0.40
2:N:223:ASN:O	2:N:497:GLN:NE2	2.54	0.40
2:N:283:ASN:O	2:N:284:LEU:HD12	2.21	0.40
1:P:192:ASP:OD2	1:P:199:GLY:HA2	2.20	0.40
1:P:320:ILE:O	1:P:322:GLY:N	2.54	0.40
2:Q:262:LEU:HA	2:Q:262:LEU:HD23	1.87	0.40
1:P:721:CYS:HB3	2:Q:446:TYR:CD2	2.56	0.40
3:R:250:LEU:HB2	3:R:270:PHE:CE2	2.51	0.40
1:D:320:ILE:O	1:D:322:GLY:N	2.54	0.40
1:D:421:ILE:HA	1:D:440:HIS:O	2.21	0.40
2:E:286:LEU:HD13	2:E:300:ASN:HD22	1.86	0.40
3:F:168:ILE:HD11	3:F:172:LYS:HE2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:56:ASP:O	1:G:57:LEU:HD13	2.21	0.40
1:G:599:LYS:HG2	2:H:272:GLN:NE2	2.36	0.40
1:G:675:PHE:HZ	1:G:742:TRP:CZ3	2.40	0.40
2:H:283:ASN:O	2:H:284:LEU:HD12	2.20	0.40
2:H:356:VAL:HG11	3:I:208:TYR:CD1	2.56	0.40
3:I:152:ILE:HG13	3:I:153:ASN:N	2.36	0.40
3:I:364:VAL:HA	3:I:367:ILE:HB	2.02	0.40
1:J:347:LEU:H	1:J:347:LEU:HD12	1.86	0.40
1:J:444:PRO:HG2	1:J:449:LEU:HD11	2.02	0.40
1:J:61:VAL:HB	1:J:551:ALA:HB3	2.03	0.40
2:K:374:THR:O	2:K:377:PHE:HB3	2.21	0.40
1:J:721:CYS:HB3	2:K:446:TYR:CD2	2.56	0.40
1:M:394:VAL:HG22	1:M:434:ARG:NH1	2.36	0.40
1:M:411:LYS:HB3	1:M:411:LYS:HE3	2.00	0.40
1:M:580:ASN:HB2	2:N:506:LYS:HE2	2.03	0.40
1:M:776:ASP:OD1	2:N:134:LYS:HE3	2.20	0.40
2:N:374:THR:HG23	3:O:219:LEU:HD13	2.03	0.40
1:P:246:LYS:HD2	1:P:303:VAL:O	2.21	0.40
2:Q:159:THR:O	2:Q:163:SER:HB2	2.22	0.40
1:A:362:ARG:HH22	1:A:364:GLU:HG3	1.86	0.40
3:C:152:ILE:HG13	3:C:153:ASN:N	2.36	0.40
3:C:236:PHE:CZ	3:C:253:ILE:HB	2.55	0.40
3:C:410:TYR:O	3:C:413:THR:OG1	2.27	0.40
1:D:304:ASP:HB2	1:D:363:ILE:O	2.20	0.40
2:E:128:GLU:O	2:E:132:VAL:HG23	2.21	0.40
2:E:374:THR:O	2:E:377:PHE:HB3	2.21	0.40
1:G:290:GLU:OE2	1:G:291:PRO:HD2	2.21	0.40
1:G:317:ILE:HD11	1:G:326:ILE:HG23	2.03	0.40
2:H:412:LYS:O	2:H:416:ILE:HG13	2.21	0.40
2:H:507:ASN:O	2:H:511:HIS:HB2	2.21	0.40
1:G:443:ASP:O	3:I:3:GLU:N	2.55	0.40
1:J:320:ILE:O	1:J:322:GLY:N	2.54	0.40
1:J:580:ASN:HB2	2:K:506:LYS:HE2	2.03	0.40
3:L:231:LEU:HD22	3:L:235:ILE:HD11	2.04	0.40
3:L:275:CYS:O	3:L:279:SER:HB3	2.21	0.40
1:M:637:LEU:HD22	1:M:637:LEU:HA	1.81	0.40
1:M:656:HIS:HE1	2:N:171:HIS:CE1	2.37	0.40
2:N:413:LEU:HA	2:N:416:ILE:HD12	2.03	0.40
3:O:305:THR:HB	3:O:308:PHE:CE1	2.55	0.40
1:P:317:ILE:CG1	1:P:326:ILE:HD13	2.51	0.40
1:P:433:VAL:HG22	1:P:434:ARG:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:56:ASP:O	1:P:57:LEU:HD13	2.22	0.40
1:P:768:TYR:O	1:P:771:ILE:HB	2.22	0.40
2:Q:128:GLU:O	2:Q:132:VAL:HG23	2.21	0.40
2:Q:226:LEU:O	2:Q:230:ILE:HG23	2.22	0.40
3:R:231:LEU:HD22	3:R:235:ILE:HD11	2.03	0.40
1:A:411:LYS:HE3	1:A:411:LYS:HB3	2.00	0.40
1:A:625:ASP:O	1:A:629:ARG:HB2	2.21	0.40
3:C:365:TRP:HB3	3:C:418:CYS:HB2	2.03	0.40
1:D:347:LEU:H	1:D:347:LEU:HD12	1.86	0.40
1:D:468:VAL:HG13	1:D:477:TYR:O	2.21	0.40
1:D:56:ASP:O	1:D:57:LEU:HD13	2.21	0.40
2:E:160:SER:HA	2:E:163:SER:HB2	2.02	0.40
2:E:177:TYR:CD1	2:E:252:LEU:HD12	2.56	0.40
1:G:185:GLN:HG3	1:G:186:TYR:H	1.85	0.40
1:G:394:VAL:HG22	1:G:434:ARG:NH1	2.37	0.40
2:H:120:ILE:HA	2:H:125:PHE:HB2	2.03	0.40
2:H:128:GLU:O	2:H:132:VAL:HG23	2.22	0.40
2:H:159:THR:O	2:H:163:SER:HB2	2.21	0.40
2:H:286:LEU:CD2	2:H:300:ASN:HB3	2.50	0.40
2:H:286:LEU:HD13	2:H:300:ASN:HD22	1.87	0.40
2:H:375:LEU:HD23	2:H:375:LEU:HA	1.93	0.40
3:I:34:ILE:HA	3:I:34:ILE:HD12	1.89	0.40
1:J:185:GLN:HG3	1:J:186:TYR:N	2.36	0.40
1:J:408:ILE:HG23	1:J:413:GLY:C	2.41	0.40
3:L:23:TYR:CZ	3:L:27:ILE:HG13	2.56	0.40
3:L:364:VAL:HA	3:L:367:ILE:HB	2.03	0.40
2:N:109:GLN:CD	2:N:137:TRP:HE1	2.21	0.40
2:N:226:LEU:O	2:N:230:ILE:HG23	2.21	0.40
2:N:313:THR:O	2:N:317:MET:HB2	2.21	0.40
2:N:410:ARG:HA	2:N:413:LEU:CB	2.46	0.40
2:N:439:ILE:HG13	2:N:439:ILE:H	1.65	0.40
2:N:507:ASN:O	2:N:511:HIS:HB2	2.22	0.40
1:M:55:LEU:HD23	3:O:227:HIS:CG	2.57	0.40
3:O:23:TYR:CZ	3:O:27:ILE:HG13	2.57	0.40
1:P:444:PRO:CG	1:P:449:LEU:HD11	2.52	0.40
2:Q:262:LEU:HD23	2:Q:334:LEU:HD21	2.02	0.40
2:Q:374:THR:O	2:Q:377:PHE:HB3	2.21	0.40
2:Q:435:GLN:HG3	2:Q:435:GLN:H	1.41	0.40
3:R:302:ARG:H	3:R:302:ARG:HG2	1.45	0.40
1:A:720:GLN:O	1:A:723:VAL:HG12	2.20	0.40
2:B:134:LYS:HA	2:B:134:LYS:HD3	1.79	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:137:SER:HA	3:C:426:VAL:HG13	2.04	0.40
1:D:411:LYS:HE3	1:D:411:LYS:HB3	2.00	0.40
1:D:444:PRO:HG2	1:D:449:LEU:HD11	2.03	0.40
1:D:474:LYS:HA	1:D:505:PRO:HD2	2.03	0.40
1:D:574:TRP:HB3	1:D:578:PHE:CE2	2.56	0.40
2:E:221:PRO:HD2	2:E:222:PHE:HD2	1.87	0.40
2:E:286:LEU:CD2	2:E:300:ASN:HB3	2.50	0.40
2:E:341:ARG:HD3	2:E:373:GLU:OE2	2.22	0.40
1:G:347:LEU:HD12	1:G:347:LEU:H	1.85	0.40
1:G:421:ILE:HA	1:G:440:HIS:O	2.22	0.40
1:G:474:LYS:HA	1:G:505:PRO:HD2	2.04	0.40
1:G:580:ASN:HB2	2:H:506:LYS:HE2	2.03	0.40
3:I:304:HIS:CD2	3:I:306:ALA:HA	2.56	0.40
1:J:394:VAL:HG22	1:J:434:ARG:NH1	2.36	0.40
1:J:768:TYR:O	1:J:771:ILE:HB	2.22	0.40
2:K:310:PHE:O	2:K:314:ILE:HG13	2.21	0.40
3:L:21:TYR:HD2	3:L:78:ARG:HB3	1.87	0.40
1:M:377:ARG:H	1:M:377:ARG:HG3	1.56	0.40
1:M:444:PRO:CG	1:M:449:LEU:HD11	2.52	0.40
1:M:61:VAL:HB	1:M:551:ALA:HB3	2.02	0.40
1:M:762:ARG:NE	1:M:762:ARG:HA	2.36	0.40
2:N:303:GLU:O	2:N:306:VAL:N	2.53	0.40
2:N:412:LYS:O	2:N:416:ILE:HG13	2.22	0.40
3:O:80:ARG:HA	3:O:83:HIS:HB3	2.04	0.40
1:P:305:PHE:HA	1:P:315:PHE:O	2.22	0.40
2:Q:341:ARG:HD3	2:Q:373:GLU:OE2	2.20	0.40
2:Q:410:ARG:HE	2:Q:413:LEU:HD13	1.86	0.40
3:R:273:TRP:CZ3	3:R:274:MET:HG2	2.55	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	584/894 (65%)	499 (85%)	65 (11%)	20 (3%)	4	27
1	D	584/894 (65%)	500 (86%)	63 (11%)	21 (4%)	4	26
1	G	584/894 (65%)	500 (86%)	62 (11%)	22 (4%)	3	24
1	J	584/894 (65%)	500 (86%)	62 (11%)	22 (4%)	3	24
1	M	584/894 (65%)	498 (85%)	65 (11%)	21 (4%)	4	26
1	P	584/894 (65%)	499 (85%)	65 (11%)	20 (3%)	4	27
2	B	367/514 (71%)	323 (88%)	40 (11%)	4 (1%)	16	56
2	E	367/514 (71%)	321 (88%)	42 (11%)	4 (1%)	16	56
2	H	367/514 (71%)	320 (87%)	43 (12%)	4 (1%)	16	56
2	K	367/514 (71%)	322 (88%)	41 (11%)	4 (1%)	16	56
2	N	367/514 (71%)	322 (88%)	41 (11%)	4 (1%)	16	56
2	Q	367/514 (71%)	321 (88%)	42 (11%)	4 (1%)	16	56
3	C	291/507 (57%)	244 (84%)	40 (14%)	7 (2%)	6	37
3	F	291/507 (57%)	248 (85%)	37 (13%)	6 (2%)	8	40
3	I	291/507 (57%)	246 (84%)	39 (13%)	6 (2%)	8	40
3	L	291/507 (57%)	246 (84%)	39 (13%)	6 (2%)	8	40
3	O	291/507 (57%)	245 (84%)	39 (13%)	7 (2%)	6	37
3	R	291/507 (57%)	248 (85%)	37 (13%)	6 (2%)	8	40
All	All	7452/11490 (65%)	6402 (86%)	862 (12%)	188 (2%)	6	36

All (188) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	321	LYS
1	A	332	ASN
1	A	444	PRO
1	A	501	PRO
1	A	752	LEU
3	C	155	GLN
3	C	427	PRO
1	D	321	LYS
1	D	332	ASN
1	D	444	PRO
1	D	501	PRO
1	D	752	LEU
3	F	155	GLN
3	F	427	PRO

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Mol	Chain	Res	Type
1	G	321	LYS
1	G	332	ASN
1	G	444	PRO
1	G	501	PRO
1	G	752	LEU
3	I	155	GLN
3	I	427	PRO
1	J	321	LYS
1	J	332	ASN
1	J	444	PRO
1	J	501	PRO
1	J	752	LEU
3	L	155	GLN
3	L	427	PRO
1	M	321	LYS
1	M	332	ASN
1	M	444	PRO
1	M	501	PRO
1	M	752	LEU
3	O	155	GLN
3	O	427	PRO
1	P	321	LYS
1	P	332	ASN
1	P	444	PRO
1	P	501	PRO
1	P	752	LEU
3	R	155	GLN
3	R	427	PRO
1	A	426	ALA
1	A	581	ALA
1	A	777	MET
2	B	362	THR
3	C	361	ASP
3	C	426	VAL
1	D	426	ALA
1	D	581	ALA
1	D	777	MET
2	E	362	THR
3	F	361	ASP
3	F	426	VAL
1	G	426	ALA
1	G	581	ALA

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Mol	Chain	Res	Type
1	G	777	MET
2	H	362	THR
3	I	361	ASP
3	I	426	VAL
1	J	426	ALA
1	J	581	ALA
1	J	777	MET
2	K	362	THR
3	L	361	ASP
3	L	426	VAL
1	M	426	ALA
1	M	581	ALA
1	M	777	MET
2	N	362	THR
3	O	361	ASP
3	O	426	VAL
1	P	426	ALA
1	P	581	ALA
1	P	777	MET
2	Q	362	THR
3	R	361	ASP
3	R	426	VAL
1	A	281	SER
1	A	411	LYS
1	A	446	ASP
2	B	148	PRO
1	D	281	SER
1	D	411	LYS
1	D	446	ASP
1	D	656	HIS
2	E	148	PRO
1	G	281	SER
1	G	411	LYS
1	G	446	ASP
1	G	656	HIS
2	H	148	PRO
1	J	281	SER
1	J	411	LYS
1	J	446	ASP
1	J	656	HIS
2	K	148	PRO
1	M	281	SER

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Mol	Chain	Res	Type
1	M	411	LYS
1	M	446	ASP
1	M	656	HIS
2	N	148	PRO
1	P	281	SER
1	P	411	LYS
1	P	446	ASP
1	P	656	HIS
2	Q	148	PRO
1	A	51	ALA
1	A	656	HIS
1	A	660	LYS
1	A	747	LEU
2	B	196	SER
1	D	51	ALA
1	D	660	LYS
1	D	747	LEU
2	E	196	SER
1	G	51	ALA
1	G	660	LYS
1	G	747	LEU
3	I	249	SER
1	J	51	ALA
1	J	660	LYS
1	J	747	LEU
2	K	196	SER
1	M	51	ALA
1	M	660	LYS
1	M	666	SER
1	M	747	LEU
2	N	196	SER
1	P	660	LYS
1	P	747	LEU
1	A	661	ASN
1	A	666	SER
3	C	249	SER
1	D	661	ASN
1	D	666	SER
3	F	249	SER
1	G	661	ASN
1	G	666	SER
2	H	196	SER

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Mol	Chain	Res	Type
1	J	568	ILE
1	J	661	ASN
1	J	666	SER
3	L	249	SER
1	M	661	ASN
3	O	249	SER
1	P	51	ALA
1	P	661	ASN
1	P	666	SER
2	Q	196	SER
3	R	249	SER
1	A	421	ILE
1	A	568	ILE
1	D	421	ILE
1	D	568	ILE
1	D	745	ALA
1	G	568	ILE
1	G	745	ALA
1	G	778	ASP
1	J	421	ILE
1	J	745	ALA
1	J	778	ASP
1	M	568	ILE
1	M	778	ASP
1	P	568	ILE
1	G	421	ILE
1	M	421	ILE
1	P	421	ILE
3	C	295	PRO
3	F	295	PRO
3	I	295	PRO
3	L	295	PRO
3	O	295	PRO
3	R	295	PRO
1	A	61	VAL
2	B	451	PRO
2	E	451	PRO
1	G	61	VAL
2	H	451	PRO
2	K	451	PRO
1	M	61	VAL
2	N	451	PRO

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Mol	Chain	Res	Type
1	P	61	VAL
2	Q	451	PRO
3	C	422	GLY
1	D	61	VAL
1	J	61	VAL
3	O	422	GLY

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	552/828 (67%)	423 (77%)	129 (23%)	1	3
1	D	552/828 (67%)	422 (76%)	130 (24%)	1	3
1	G	552/828 (67%)	425 (77%)	127 (23%)	1	4
1	J	552/828 (67%)	424 (77%)	128 (23%)	1	4
1	M	552/828 (67%)	424 (77%)	128 (23%)	1	4
1	P	552/828 (67%)	425 (77%)	127 (23%)	1	4
2	B	354/476 (74%)	298 (84%)	56 (16%)	3	13
2	E	354/476 (74%)	297 (84%)	57 (16%)	2	12
2	H	354/476 (74%)	297 (84%)	57 (16%)	2	12
2	K	354/476 (74%)	297 (84%)	57 (16%)	2	12
2	N	354/476 (74%)	297 (84%)	57 (16%)	2	12
2	Q	354/476 (74%)	297 (84%)	57 (16%)	2	12
3	C	286/474 (60%)	221 (77%)	65 (23%)	1	4
3	F	286/474 (60%)	221 (77%)	65 (23%)	1	4
3	I	286/474 (60%)	220 (77%)	66 (23%)	1	4
3	L	286/474 (60%)	222 (78%)	64 (22%)	1	4
3	O	286/474 (60%)	220 (77%)	66 (23%)	1	4
3	R	286/474 (60%)	221 (77%)	65 (23%)	1	4
All	All	7152/10668 (67%)	5651 (79%)	1501 (21%)	1	6

All (1501) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	GLN
1	A	26	TYR
1	A	49	THR
1	A	52	GLU
1	A	55	LEU
1	A	64	LEU
1	A	200	THR
1	A	214	LEU
1	A	218	VAL
1	A	236	ILE
1	A	247	ILE
1	A	252	GLU
1	A	260	LEU
1	A	273	ARG
1	A	286	VAL
1	A	289	SER
1	A	290	GLU
1	A	292	LEU
1	A	295	VAL
1	A	300	LEU
1	A	314	GLN
1	A	321	LYS
1	A	329	ILE
1	A	331	LYS
1	A	333	PHE
1	A	343	LEU
1	A	345	ASP
1	A	347	LEU
1	A	355	GLU
1	A	356	GLU
1	A	359	SER
1	A	360	TRP
1	A	363	ILE
1	A	364	GLU
1	A	369	PHE
1	A	377	ARG
1	A	378	SER
1	A	379	LYS
1	A	381	ILE
1	A	384	ASP
1	A	386	MET
1	A	390	GLN

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Mol	Chain	Res	Type
1	A	403	ARG
1	A	407	ARG
1	A	408	ILE
1	A	410	ASP
1	A	412	ASN
1	A	415	LEU
1	A	417	THR
1	A	419	ARG
1	A	421	ILE
1	A	424	VAL
1	A	430	ASN
1	A	433	VAL
1	A	434	ARG
1	A	439	LYS
1	A	442	LEU
1	A	443	ASP
1	A	448	THR
1	A	453	VAL
1	A	455	LYS
1	A	460	ASP
1	A	463	LEU
1	A	464	LEU
1	A	465	VAL
1	A	473	HIS
1	A	474	LYS
1	A	492	LEU
1	A	494	CYS
1	A	496	THR
1	A	497	VAL
1	A	498	LEU
1	A	500	ILE
1	A	508	ILE
1	A	511	ILE
1	A	531	PHE
1	A	534	VAL
1	A	538	LEU
1	A	539	VAL
1	A	545	SER
1	A	555	THR
1	A	556	GLN
1	A	574	TRP
1	A	580	ASN

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Mol	Chain	Res	Type
1	A	582	ASP
1	A	584	ARG
1	A	596	ILE
1	A	600	GLU
1	A	609	ASN
1	A	615	ASN
1	A	617	HIS
1	A	625	ASP
1	A	626	LEU
1	A	630	LEU
1	A	632	ILE
1	A	635	ASN
1	A	637	LEU
1	A	638	LEU
1	A	646	ASP
1	A	647	GLU
1	A	654	LEU
1	A	656	HIS
1	A	659	LEU
1	A	660	LYS
1	A	662	LEU
1	A	665	ASN
1	A	667	ASP
1	A	671	SER
1	A	676	SER
1	A	679	LEU
1	A	693	PHE
1	A	700	LEU
1	A	706	GLU
1	A	711	LEU
1	A	712	ASP
1	A	726	SER
1	A	730	GLU
1	A	731	LEU
1	A	736	ILE
1	A	742	TRP
1	A	748	GLU
1	A	749	LYS
1	A	751	SER
1	A	753	PHE
1	A	757	GLN
1	A	762	ARG

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Mol	Chain	Res	Type
1	A	768	TYR
1	A	772	ILE
1	A	777	MET
2	B	103	LEU
2	B	110	PHE
2	B	112	LEU
2	B	138	LEU
2	B	139	LYS
2	B	143	THR
2	B	145	ASN
2	B	147	GLN
2	B	154	LEU
2	B	159	THR
2	B	163	SER
2	B	164	ILE
2	B	167	LEU
2	B	169	SER
2	B	173	SER
2	B	176	VAL
2	B	187	THR
2	B	204	ARG
2	B	207	LEU
2	B	220	SER
2	B	226	LEU
2	B	229	LYS
2	B	232	LEU
2	B	248	SER
2	B	273	VAL
2	B	290	THR
2	B	291	ASP
2	B	292	GLU
2	B	301	HIS
2	B	312	LEU
2	B	323	ASP
2	B	328	LEU
2	B	332	LEU
2	B	337	SER
2	B	348	ILE
2	B	359	ASP
2	B	363	SER
2	B	366	TYR
2	B	367	PHE

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Mol	Chain	Res	Type
2	B	379	LYS
2	B	384	GLN
2	B	389	GLN
2	B	419	LEU
2	B	432	SER
2	B	434	HIS
2	B	435	GLN
2	B	436	LEU
2	B	444	GLU
2	B	445	ARG
2	B	453	PHE
2	B	495	LYS
2	B	502	ILE
2	B	506	LYS
2	B	511	HIS
2	B	512	ARG
2	B	513	MET
3	C	1	MET
3	C	4	VAL
3	C	8	LEU
3	C	9	THR
3	C	10	ASN
3	C	11	ARG
3	C	15	GLN
3	C	74	GLN
3	C	84	TRP
3	C	85	ARG
3	C	87	VAL
3	C	141	TRP
3	C	143	THR
3	C	149	LYS
3	C	150	GLN
3	C	156	LYS
3	C	158	THR
3	C	160	HIS
3	C	168	ILE
3	C	178	LEU
3	C	196	GLU
3	C	198	LEU
3	C	202	THR
3	C	209	ARG
3	C	210	THR

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Mol	Chain	Res	Type
3	C	211	ARG
3	C	212	HIS
3	C	216	LEU
3	C	218	ASP
3	C	230	SER
3	C	231	LEU
3	C	235	ILE
3	C	238	THR
3	C	242	ILE
3	C	247	ILE
3	C	248	LYS
3	C	250	LEU
3	C	255	VAL
3	C	264	SER
3	C	266	SER
3	C	269	ASP
3	C	272	GLN
3	C	298	GLN
3	C	299	THR
3	C	302	ARG
3	C	307	LYS
3	C	308	PHE
3	C	312	TYR
3	C	313	LEU
3	C	322	LYS
3	C	323	SER
3	C	345	LEU
3	C	347	ASP
3	C	360	GLU
3	C	364	VAL
3	C	367	ILE
3	C	368	TYR
3	C	373	LEU
3	C	374	LEU
3	C	402	ASN
3	C	410	TYR
3	C	415	LEU
3	C	420	ASP
3	C	429	ARG
3	C	430	LEU
1	D	21	GLN
1	D	26	TYR

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Mol	Chain	Res	Type
1	D	49	THR
1	D	52	GLU
1	D	55	LEU
1	D	64	LEU
1	D	200	THR
1	D	214	LEU
1	D	218	VAL
1	D	236	ILE
1	D	247	ILE
1	D	252	GLU
1	D	260	LEU
1	D	273	ARG
1	D	286	VAL
1	D	289	SER
1	D	290	GLU
1	D	292	LEU
1	D	295	VAL
1	D	300	LEU
1	D	314	GLN
1	D	321	LYS
1	D	329	ILE
1	D	331	LYS
1	D	333	PHE
1	D	343	LEU
1	D	345	ASP
1	D	347	LEU
1	D	355	GLU
1	D	356	GLU
1	D	359	SER
1	D	360	TRP
1	D	363	ILE
1	D	364	GLU
1	D	369	PHE
1	D	377	ARG
1	D	378	SER
1	D	379	LYS
1	D	381	ILE
1	D	384	ASP
1	D	386	MET
1	D	390	GLN
1	D	403	ARG
1	D	407	ARG

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Mol	Chain	Res	Type
1	D	408	ILE
1	D	410	ASP
1	D	412	ASN
1	D	415	LEU
1	D	417	THR
1	D	419	ARG
1	D	421	ILE
1	D	424	VAL
1	D	430	ASN
1	D	433	VAL
1	D	434	ARG
1	D	439	LYS
1	D	442	LEU
1	D	443	ASP
1	D	448	THR
1	D	453	VAL
1	D	455	LYS
1	D	460	ASP
1	D	463	LEU
1	D	464	LEU
1	D	465	VAL
1	D	473	HIS
1	D	474	LYS
1	D	492	LEU
1	D	494	CYS
1	D	495	SER
1	D	496	THR
1	D	497	VAL
1	D	498	LEU
1	D	500	ILE
1	D	508	ILE
1	D	511	ILE
1	D	531	PHE
1	D	534	VAL
1	D	538	LEU
1	D	539	VAL
1	D	545	SER
1	D	555	THR
1	D	556	GLN
1	D	574	TRP
1	D	580	ASN
1	D	582	ASP

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Mol	Chain	Res	Type
1	D	584	ARG
1	D	596	ILE
1	D	600	GLU
1	D	609	ASN
1	D	615	ASN
1	D	617	HIS
1	D	625	ASP
1	D	626	LEU
1	D	630	LEU
1	D	632	ILE
1	D	635	ASN
1	D	637	LEU
1	D	638	LEU
1	D	646	ASP
1	D	647	GLU
1	D	654	LEU
1	D	656	HIS
1	D	659	LEU
1	D	660	LYS
1	D	662	LEU
1	D	665	ASN
1	D	667	ASP
1	D	671	SER
1	D	676	SER
1	D	679	LEU
1	D	693	PHE
1	D	700	LEU
1	D	706	GLU
1	D	711	LEU
1	D	712	ASP
1	D	726	SER
1	D	730	GLU
1	D	731	LEU
1	D	736	ILE
1	D	742	TRP
1	D	748	GLU
1	D	749	LYS
1	D	751	SER
1	D	753	PHE
1	D	757	GLN
1	D	762	ARG
1	D	768	TYR

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Mol	Chain	Res	Type
1	D	772	ILE
1	D	777	MET
2	E	103	LEU
2	E	110	PHE
2	E	112	LEU
2	E	119	LEU
2	E	138	LEU
2	E	139	LYS
2	E	143	THR
2	E	145	ASN
2	E	147	GLN
2	E	154	LEU
2	E	159	THR
2	E	163	SER
2	E	164	ILE
2	E	167	LEU
2	E	169	SER
2	E	173	SER
2	E	176	VAL
2	E	187	THR
2	E	204	ARG
2	E	207	LEU
2	E	220	SER
2	E	226	LEU
2	E	229	LYS
2	E	232	LEU
2	E	248	SER
2	E	273	VAL
2	E	290	THR
2	E	291	ASP
2	E	292	GLU
2	E	301	HIS
2	E	312	LEU
2	E	323	ASP
2	E	328	LEU
2	E	332	LEU
2	E	337	SER
2	E	348	ILE
2	E	359	ASP
2	E	363	SER
2	E	366	TYR
2	E	367	PHE

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Mol	Chain	Res	Type
2	E	379	LYS
2	E	384	GLN
2	E	389	GLN
2	E	419	LEU
2	E	432	SER
2	E	434	HIS
2	E	435	GLN
2	E	436	LEU
2	E	444	GLU
2	E	445	ARG
2	E	453	PHE
2	E	495	LYS
2	E	502	ILE
2	E	506	LYS
2	E	511	HIS
2	E	512	ARG
2	E	513	MET
3	F	1	MET
3	F	4	VAL
3	F	8	LEU
3	F	10	ASN
3	F	11	ARG
3	F	15	GLN
3	F	74	GLN
3	F	84	TRP
3	F	85	ARG
3	F	87	VAL
3	F	141	TRP
3	F	143	THR
3	F	149	LYS
3	F	150	GLN
3	F	156	LYS
3	F	158	THR
3	F	160	HIS
3	F	168	ILE
3	F	178	LEU
3	F	196	GLU
3	F	198	LEU
3	F	202	THR
3	F	209	ARG
3	F	210	THR
3	F	211	ARG

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Mol	Chain	Res	Type
3	F	212	HIS
3	F	216	LEU
3	F	218	ASP
3	F	230	SER
3	F	231	LEU
3	F	235	ILE
3	F	238	THR
3	F	242	ILE
3	F	247	ILE
3	F	248	LYS
3	F	250	LEU
3	F	255	VAL
3	F	264	SER
3	F	266	SER
3	F	269	ASP
3	F	272	GLN
3	F	298	GLN
3	F	299	THR
3	F	302	ARG
3	F	307	LYS
3	F	308	PHE
3	F	312	TYR
3	F	313	LEU
3	F	319	ASN
3	F	322	LYS
3	F	323	SER
3	F	345	LEU
3	F	347	ASP
3	F	360	GLU
3	F	364	VAL
3	F	367	ILE
3	F	368	TYR
3	F	373	LEU
3	F	374	LEU
3	F	402	ASN
3	F	410	TYR
3	F	415	LEU
3	F	420	ASP
3	F	429	ARG
3	F	430	LEU
1	G	21	GLN
1	G	26	TYR

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Mol	Chain	Res	Type
1	G	49	THR
1	G	52	GLU
1	G	55	LEU
1	G	64	LEU
1	G	200	THR
1	G	214	LEU
1	G	218	VAL
1	G	236	ILE
1	G	247	ILE
1	G	252	GLU
1	G	260	LEU
1	G	273	ARG
1	G	286	VAL
1	G	290	GLU
1	G	292	LEU
1	G	295	VAL
1	G	300	LEU
1	G	314	GLN
1	G	321	LYS
1	G	329	ILE
1	G	331	LYS
1	G	333	PHE
1	G	343	LEU
1	G	345	ASP
1	G	347	LEU
1	G	355	GLU
1	G	356	GLU
1	G	359	SER
1	G	360	TRP
1	G	363	ILE
1	G	364	GLU
1	G	369	PHE
1	G	377	ARG
1	G	378	SER
1	G	379	LYS
1	G	381	ILE
1	G	384	ASP
1	G	386	MET
1	G	390	GLN
1	G	403	ARG
1	G	407	ARG
1	G	408	ILE

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Mol	Chain	Res	Type
1	G	410	ASP
1	G	412	ASN
1	G	415	LEU
1	G	417	THR
1	G	419	ARG
1	G	421	ILE
1	G	424	VAL
1	G	430	ASN
1	G	433	VAL
1	G	434	ARG
1	G	439	LYS
1	G	442	LEU
1	G	443	ASP
1	G	448	THR
1	G	453	VAL
1	G	455	LYS
1	G	460	ASP
1	G	463	LEU
1	G	464	LEU
1	G	465	VAL
1	G	473	HIS
1	G	474	LYS
1	G	492	LEU
1	G	494	CYS
1	G	496	THR
1	G	497	VAL
1	G	498	LEU
1	G	500	ILE
1	G	511	ILE
1	G	531	PHE
1	G	534	VAL
1	G	538	LEU
1	G	539	VAL
1	G	545	SER
1	G	555	THR
1	G	556	GLN
1	G	574	TRP
1	G	580	ASN
1	G	582	ASP
1	G	584	ARG
1	G	596	ILE
1	G	600	GLU

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Mol	Chain	Res	Type
1	G	609	ASN
1	G	615	ASN
1	G	617	HIS
1	G	625	ASP
1	G	626	LEU
1	G	630	LEU
1	G	632	ILE
1	G	635	ASN
1	G	637	LEU
1	G	638	LEU
1	G	646	ASP
1	G	647	GLU
1	G	654	LEU
1	G	656	HIS
1	G	659	LEU
1	G	660	LYS
1	G	662	LEU
1	G	665	ASN
1	G	667	ASP
1	G	671	SER
1	G	676	SER
1	G	679	LEU
1	G	693	PHE
1	G	700	LEU
1	G	706	GLU
1	G	711	LEU
1	G	712	ASP
1	G	726	SER
1	G	730	GLU
1	G	731	LEU
1	G	736	ILE
1	G	742	TRP
1	G	748	GLU
1	G	749	LYS
1	G	751	SER
1	G	753	PHE
1	G	757	GLN
1	G	762	ARG
1	G	768	TYR
1	G	772	ILE
1	G	777	MET
2	H	103	LEU

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Mol	Chain	Res	Type
2	H	110	PHE
2	H	112	LEU
2	H	119	LEU
2	H	138	LEU
2	H	139	LYS
2	H	143	THR
2	H	145	ASN
2	H	147	GLN
2	H	154	LEU
2	H	159	THR
2	H	163	SER
2	H	164	ILE
2	H	167	LEU
2	H	169	SER
2	H	173	SER
2	H	176	VAL
2	H	187	THR
2	H	204	ARG
2	H	207	LEU
2	H	220	SER
2	H	226	LEU
2	H	229	LYS
2	H	232	LEU
2	H	248	SER
2	H	273	VAL
2	H	290	THR
2	H	291	ASP
2	H	292	GLU
2	H	301	HIS
2	H	312	LEU
2	H	323	ASP
2	H	328	LEU
2	H	332	LEU
2	H	337	SER
2	H	348	ILE
2	H	359	ASP
2	H	363	SER
2	H	366	TYR
2	H	367	PHE
2	H	379	LYS
2	H	384	GLN
2	H	389	GLN

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Mol	Chain	Res	Type
2	H	419	LEU
2	H	432	SER
2	H	434	HIS
2	H	435	GLN
2	H	436	LEU
2	H	444	GLU
2	H	445	ARG
2	H	453	PHE
2	H	495	LYS
2	H	502	ILE
2	H	506	LYS
2	H	511	HIS
2	H	512	ARG
2	H	513	MET
3	I	1	MET
3	I	4	VAL
3	I	8	LEU
3	I	9	THR
3	I	10	ASN
3	I	11	ARG
3	I	15	GLN
3	I	74	GLN
3	I	84	TRP
3	I	85	ARG
3	I	87	VAL
3	I	141	TRP
3	I	143	THR
3	I	149	LYS
3	I	150	GLN
3	I	156	LYS
3	I	158	THR
3	I	160	HIS
3	I	168	ILE
3	I	178	LEU
3	I	196	GLU
3	I	198	LEU
3	I	202	THR
3	I	209	ARG
3	I	210	THR
3	I	211	ARG
3	I	212	HIS
3	I	216	LEU

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Mol	Chain	Res	Type
3	I	218	ASP
3	I	230	SER
3	I	231	LEU
3	I	235	ILE
3	I	238	THR
3	I	242	ILE
3	I	247	ILE
3	I	248	LYS
3	I	250	LEU
3	I	255	VAL
3	I	264	SER
3	I	266	SER
3	I	269	ASP
3	I	272	GLN
3	I	298	GLN
3	I	299	THR
3	I	302	ARG
3	I	307	LYS
3	I	308	PHE
3	I	312	TYR
3	I	313	LEU
3	I	319	ASN
3	I	322	LYS
3	I	323	SER
3	I	345	LEU
3	I	347	ASP
3	I	360	GLU
3	I	364	VAL
3	I	367	ILE
3	I	368	TYR
3	I	373	LEU
3	I	374	LEU
3	I	402	ASN
3	I	410	TYR
3	I	415	LEU
3	I	420	ASP
3	I	429	ARG
3	I	430	LEU
1	J	21	GLN
1	J	26	TYR
1	J	49	THR
1	J	52	GLU

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Mol	Chain	Res	Type
1	J	55	LEU
1	J	64	LEU
1	J	200	THR
1	J	214	LEU
1	J	218	VAL
1	J	236	ILE
1	J	247	ILE
1	J	252	GLU
1	J	260	LEU
1	J	273	ARG
1	J	286	VAL
1	J	289	SER
1	J	290	GLU
1	J	292	LEU
1	J	295	VAL
1	J	300	LEU
1	J	314	GLN
1	J	321	LYS
1	J	329	ILE
1	J	331	LYS
1	J	333	PHE
1	J	343	LEU
1	J	345	ASP
1	J	347	LEU
1	J	355	GLU
1	J	356	GLU
1	J	359	SER
1	J	360	TRP
1	J	363	ILE
1	J	364	GLU
1	J	369	PHE
1	J	377	ARG
1	J	378	SER
1	J	379	LYS
1	J	381	ILE
1	J	384	ASP
1	J	386	MET
1	J	390	GLN
1	J	403	ARG
1	J	407	ARG
1	J	408	ILE
1	J	410	ASP

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Mol	Chain	Res	Type
1	J	412	ASN
1	J	415	LEU
1	J	417	THR
1	J	419	ARG
1	J	421	ILE
1	J	424	VAL
1	J	430	ASN
1	J	433	VAL
1	J	434	ARG
1	J	439	LYS
1	J	442	LEU
1	J	443	ASP
1	J	448	THR
1	J	453	VAL
1	J	455	LYS
1	J	460	ASP
1	J	463	LEU
1	J	464	LEU
1	J	465	VAL
1	J	473	HIS
1	J	474	LYS
1	J	492	LEU
1	J	494	CYS
1	J	496	THR
1	J	497	VAL
1	J	498	LEU
1	J	500	ILE
1	J	511	ILE
1	J	531	PHE
1	J	534	VAL
1	J	538	LEU
1	J	539	VAL
1	J	545	SER
1	J	555	THR
1	J	556	GLN
1	J	574	TRP
1	J	580	ASN
1	J	582	ASP
1	J	584	ARG
1	J	596	ILE
1	J	600	GLU
1	J	609	ASN

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Mol	Chain	Res	Type
1	J	615	ASN
1	J	617	HIS
1	J	625	ASP
1	J	626	LEU
1	J	630	LEU
1	J	632	ILE
1	J	635	ASN
1	J	637	LEU
1	J	638	LEU
1	J	646	ASP
1	J	647	GLU
1	J	654	LEU
1	J	656	HIS
1	J	659	LEU
1	J	660	LYS
1	J	662	LEU
1	J	665	ASN
1	J	667	ASP
1	J	671	SER
1	J	676	SER
1	J	679	LEU
1	J	693	PHE
1	J	700	LEU
1	J	706	GLU
1	J	711	LEU
1	J	712	ASP
1	J	726	SER
1	J	730	GLU
1	J	731	LEU
1	J	736	ILE
1	J	742	TRP
1	J	748	GLU
1	J	749	LYS
1	J	751	SER
1	J	753	PHE
1	J	757	GLN
1	J	762	ARG
1	J	768	TYR
1	J	772	ILE
1	J	777	MET
2	K	103	LEU
2	K	110	PHE

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Mol	Chain	Res	Type
2	K	112	LEU
2	K	119	LEU
2	K	138	LEU
2	K	139	LYS
2	K	143	THR
2	K	145	ASN
2	K	147	GLN
2	K	154	LEU
2	K	159	THR
2	K	163	SER
2	K	164	ILE
2	K	167	LEU
2	K	169	SER
2	K	173	SER
2	K	176	VAL
2	K	187	THR
2	K	204	ARG
2	K	207	LEU
2	K	220	SER
2	K	226	LEU
2	K	229	LYS
2	K	232	LEU
2	K	248	SER
2	K	273	VAL
2	K	290	THR
2	K	291	ASP
2	K	292	GLU
2	K	301	HIS
2	K	312	LEU
2	K	323	ASP
2	K	328	LEU
2	K	332	LEU
2	K	337	SER
2	K	348	ILE
2	K	359	ASP
2	K	363	SER
2	K	366	TYR
2	K	367	PHE
2	K	379	LYS
2	K	384	GLN
2	K	389	GLN
2	K	419	LEU

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Mol	Chain	Res	Type
2	K	432	SER
2	K	434	HIS
2	K	435	GLN
2	K	436	LEU
2	K	444	GLU
2	K	445	ARG
2	K	453	PHE
2	K	495	LYS
2	K	502	ILE
2	K	506	LYS
2	K	511	HIS
2	K	512	ARG
2	K	513	MET
3	L	1	MET
3	L	4	VAL
3	L	8	LEU
3	L	10	ASN
3	L	11	ARG
3	L	15	GLN
3	L	74	GLN
3	L	84	TRP
3	L	85	ARG
3	L	87	VAL
3	L	141	TRP
3	L	143	THR
3	L	149	LYS
3	L	150	GLN
3	L	156	LYS
3	L	158	THR
3	L	160	HIS
3	L	168	ILE
3	L	178	LEU
3	L	196	GLU
3	L	198	LEU
3	L	202	THR
3	L	209	ARG
3	L	210	THR
3	L	211	ARG
3	L	212	HIS
3	L	216	LEU
3	L	218	ASP
3	L	230	SER

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Mol	Chain	Res	Type
3	L	231	LEU
3	L	235	ILE
3	L	238	THR
3	L	242	ILE
3	L	247	ILE
3	L	248	LYS
3	L	250	LEU
3	L	255	VAL
3	L	264	SER
3	L	266	SER
3	L	269	ASP
3	L	272	GLN
3	L	298	GLN
3	L	299	THR
3	L	302	ARG
3	L	307	LYS
3	L	308	PHE
3	L	312	TYR
3	L	313	LEU
3	L	322	LYS
3	L	323	SER
3	L	345	LEU
3	L	347	ASP
3	L	360	GLU
3	L	364	VAL
3	L	367	ILE
3	L	368	TYR
3	L	373	LEU
3	L	374	LEU
3	L	402	ASN
3	L	410	TYR
3	L	415	LEU
3	L	420	ASP
3	L	429	ARG
3	L	430	LEU
1	M	21	GLN
1	M	26	TYR
1	M	49	THR
1	M	52	GLU
1	M	55	LEU
1	M	64	LEU
1	M	200	THR

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Mol	Chain	Res	Type
1	M	214	LEU
1	M	218	VAL
1	M	236	ILE
1	M	247	ILE
1	M	252	GLU
1	M	260	LEU
1	M	273	ARG
1	M	286	VAL
1	M	289	SER
1	M	290	GLU
1	M	292	LEU
1	M	295	VAL
1	M	300	LEU
1	M	314	GLN
1	M	321	LYS
1	M	329	ILE
1	M	331	LYS
1	M	333	PHE
1	M	343	LEU
1	M	345	ASP
1	M	347	LEU
1	M	355	GLU
1	M	356	GLU
1	M	359	SER
1	M	360	TRP
1	M	363	ILE
1	M	364	GLU
1	M	369	PHE
1	M	377	ARG
1	M	378	SER
1	M	379	LYS
1	M	381	ILE
1	M	384	ASP
1	M	386	MET
1	M	390	GLN
1	M	403	ARG
1	M	407	ARG
1	M	408	ILE
1	M	410	ASP
1	M	412	ASN
1	M	415	LEU
1	M	417	THR

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Mol	Chain	Res	Type
1	M	419	ARG
1	M	421	ILE
1	M	424	VAL
1	M	430	ASN
1	M	433	VAL
1	M	434	ARG
1	M	439	LYS
1	M	442	LEU
1	M	443	ASP
1	M	448	THR
1	M	453	VAL
1	M	455	LYS
1	M	460	ASP
1	M	463	LEU
1	M	464	LEU
1	M	465	VAL
1	M	473	HIS
1	M	474	LYS
1	M	492	LEU
1	M	494	CYS
1	M	496	THR
1	M	497	VAL
1	M	498	LEU
1	M	500	ILE
1	M	511	ILE
1	M	531	PHE
1	M	534	VAL
1	M	538	LEU
1	M	539	VAL
1	M	545	SER
1	M	555	THR
1	M	556	GLN
1	M	574	TRP
1	M	580	ASN
1	M	582	ASP
1	M	584	ARG
1	M	596	ILE
1	M	600	GLU
1	M	609	ASN
1	M	615	ASN
1	M	617	HIS
1	M	625	ASP

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Mol	Chain	Res	Type
1	M	626	LEU
1	M	630	LEU
1	M	632	ILE
1	M	635	ASN
1	M	637	LEU
1	M	638	LEU
1	M	646	ASP
1	M	647	GLU
1	M	654	LEU
1	M	656	HIS
1	M	659	LEU
1	M	660	LYS
1	M	662	LEU
1	M	665	ASN
1	M	667	ASP
1	M	671	SER
1	M	676	SER
1	M	679	LEU
1	M	693	PHE
1	M	700	LEU
1	M	706	GLU
1	M	711	LEU
1	M	712	ASP
1	M	726	SER
1	M	730	GLU
1	M	731	LEU
1	M	736	ILE
1	M	742	TRP
1	M	748	GLU
1	M	749	LYS
1	M	751	SER
1	M	753	PHE
1	M	757	GLN
1	M	762	ARG
1	M	768	TYR
1	M	772	ILE
1	M	777	MET
2	N	103	LEU
2	N	110	PHE
2	N	112	LEU
2	N	119	LEU
2	N	138	LEU

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Mol	Chain	Res	Type
2	N	139	LYS
2	N	143	THR
2	N	145	ASN
2	N	147	GLN
2	N	154	LEU
2	N	159	THR
2	N	163	SER
2	N	164	ILE
2	N	167	LEU
2	N	169	SER
2	N	173	SER
2	N	176	VAL
2	N	187	THR
2	N	204	ARG
2	N	207	LEU
2	N	220	SER
2	N	226	LEU
2	N	229	LYS
2	N	232	LEU
2	N	248	SER
2	N	273	VAL
2	N	290	THR
2	N	291	ASP
2	N	292	GLU
2	N	301	HIS
2	N	312	LEU
2	N	323	ASP
2	N	328	LEU
2	N	332	LEU
2	N	337	SER
2	N	348	ILE
2	N	359	ASP
2	N	363	SER
2	N	366	TYR
2	N	367	PHE
2	N	379	LYS
2	N	384	GLN
2	N	389	GLN
2	N	419	LEU
2	N	432	SER
2	N	434	HIS
2	N	435	GLN

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Mol	Chain	Res	Type
2	N	436	LEU
2	N	444	GLU
2	N	445	ARG
2	N	453	PHE
2	N	495	LYS
2	N	502	ILE
2	N	506	LYS
2	N	511	HIS
2	N	512	ARG
2	N	513	MET
3	O	1	MET
3	O	4	VAL
3	O	8	LEU
3	O	9	THR
3	O	10	ASN
3	O	11	ARG
3	O	15	GLN
3	O	74	GLN
3	O	84	TRP
3	O	85	ARG
3	O	87	VAL
3	O	141	TRP
3	O	143	THR
3	O	149	LYS
3	O	150	GLN
3	O	156	LYS
3	O	158	THR
3	O	160	HIS
3	O	168	ILE
3	O	178	LEU
3	O	196	GLU
3	O	198	LEU
3	O	202	THR
3	O	209	ARG
3	O	210	THR
3	O	211	ARG
3	O	212	HIS
3	O	216	LEU
3	O	218	ASP
3	O	230	SER
3	O	231	LEU
3	O	235	ILE

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Mol	Chain	Res	Type
3	O	238	THR
3	O	242	ILE
3	O	247	ILE
3	O	248	LYS
3	O	250	LEU
3	O	255	VAL
3	O	264	SER
3	O	266	SER
3	O	269	ASP
3	O	272	GLN
3	O	298	GLN
3	O	299	THR
3	O	302	ARG
3	O	307	LYS
3	O	308	PHE
3	O	312	TYR
3	O	313	LEU
3	O	319	ASN
3	O	322	LYS
3	O	323	SER
3	O	345	LEU
3	O	347	ASP
3	O	360	GLU
3	O	364	VAL
3	O	367	ILE
3	O	368	TYR
3	O	373	LEU
3	O	374	LEU
3	O	402	ASN
3	O	410	TYR
3	O	415	LEU
3	O	420	ASP
3	O	429	ARG
3	O	430	LEU
1	P	21	GLN
1	P	26	TYR
1	P	49	THR
1	P	52	GLU
1	P	55	LEU
1	P	64	LEU
1	P	200	THR
1	P	214	LEU

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Mol	Chain	Res	Type
1	P	218	VAL
1	P	236	ILE
1	P	247	ILE
1	P	252	GLU
1	P	260	LEU
1	P	273	ARG
1	P	286	VAL
1	P	290	GLU
1	P	292	LEU
1	P	295	VAL
1	P	300	LEU
1	P	314	GLN
1	P	321	LYS
1	P	329	ILE
1	P	331	LYS
1	P	333	PHE
1	P	343	LEU
1	P	345	ASP
1	P	347	LEU
1	P	355	GLU
1	P	356	GLU
1	P	359	SER
1	P	360	TRP
1	P	363	ILE
1	P	364	GLU
1	P	369	PHE
1	P	377	ARG
1	P	378	SER
1	P	379	LYS
1	P	381	ILE
1	P	384	ASP
1	P	386	MET
1	P	390	GLN
1	P	403	ARG
1	P	407	ARG
1	P	408	ILE
1	P	410	ASP
1	P	412	ASN
1	P	415	LEU
1	P	417	THR
1	P	419	ARG
1	P	421	ILE

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Mol	Chain	Res	Type
1	P	424	VAL
1	P	430	ASN
1	P	433	VAL
1	P	434	ARG
1	P	439	LYS
1	P	442	LEU
1	P	443	ASP
1	P	448	THR
1	P	453	VAL
1	P	455	LYS
1	P	460	ASP
1	P	463	LEU
1	P	464	LEU
1	P	465	VAL
1	P	473	HIS
1	P	474	LYS
1	P	492	LEU
1	P	494	CYS
1	P	496	THR
1	P	497	VAL
1	P	498	LEU
1	P	500	ILE
1	P	511	ILE
1	P	531	PHE
1	P	534	VAL
1	P	538	LEU
1	P	539	VAL
1	P	545	SER
1	P	555	THR
1	P	556	GLN
1	P	574	TRP
1	P	580	ASN
1	P	582	ASP
1	P	584	ARG
1	P	596	ILE
1	P	600	GLU
1	P	609	ASN
1	P	615	ASN
1	P	617	HIS
1	P	625	ASP
1	P	626	LEU
1	P	630	LEU

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Mol	Chain	Res	Type
1	P	632	ILE
1	P	635	ASN
1	P	637	LEU
1	P	638	LEU
1	P	646	ASP
1	P	647	GLU
1	P	654	LEU
1	P	656	HIS
1	P	659	LEU
1	P	660	LYS
1	P	662	LEU
1	P	665	ASN
1	P	667	ASP
1	P	671	SER
1	P	676	SER
1	P	679	LEU
1	P	693	PHE
1	P	700	LEU
1	P	706	GLU
1	P	711	LEU
1	P	712	ASP
1	P	726	SER
1	P	730	GLU
1	P	731	LEU
1	P	736	ILE
1	P	742	TRP
1	P	748	GLU
1	P	749	LYS
1	P	751	SER
1	P	753	PHE
1	P	757	GLN
1	P	762	ARG
1	P	768	TYR
1	P	772	ILE
1	P	777	MET
2	Q	103	LEU
2	Q	110	PHE
2	Q	112	LEU
2	Q	119	LEU
2	Q	138	LEU
2	Q	139	LYS
2	Q	143	THR

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Mol	Chain	Res	Type
2	Q	145	ASN
2	Q	147	GLN
2	Q	154	LEU
2	Q	159	THR
2	Q	163	SER
2	Q	164	ILE
2	Q	167	LEU
2	Q	169	SER
2	Q	173	SER
2	Q	176	VAL
2	Q	187	THR
2	Q	204	ARG
2	Q	207	LEU
2	Q	220	SER
2	Q	226	LEU
2	Q	229	LYS
2	Q	232	LEU
2	Q	248	SER
2	Q	273	VAL
2	Q	290	THR
2	Q	291	ASP
2	Q	292	GLU
2	Q	301	HIS
2	Q	312	LEU
2	Q	323	ASP
2	Q	328	LEU
2	Q	332	LEU
2	Q	337	SER
2	Q	348	ILE
2	Q	359	ASP
2	Q	363	SER
2	Q	366	TYR
2	Q	367	PHE
2	Q	379	LYS
2	Q	384	GLN
2	Q	389	GLN
2	Q	419	LEU
2	Q	432	SER
2	Q	434	HIS
2	Q	435	GLN
2	Q	436	LEU
2	Q	444	GLU

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Mol	Chain	Res	Type
2	Q	445	ARG
2	Q	453	PHE
2	Q	495	LYS
2	Q	502	ILE
2	Q	506	LYS
2	Q	511	HIS
2	Q	512	ARG
2	Q	513	MET
3	R	1	MET
3	R	4	VAL
3	R	8	LEU
3	R	10	ASN
3	R	11	ARG
3	R	15	GLN
3	R	74	GLN
3	R	84	TRP
3	R	85	ARG
3	R	87	VAL
3	R	141	TRP
3	R	143	THR
3	R	149	LYS
3	R	150	GLN
3	R	156	LYS
3	R	158	THR
3	R	160	HIS
3	R	168	ILE
3	R	178	LEU
3	R	196	GLU
3	R	198	LEU
3	R	202	THR
3	R	209	ARG
3	R	210	THR
3	R	211	ARG
3	R	212	HIS
3	R	216	LEU
3	R	218	ASP
3	R	230	SER
3	R	231	LEU
3	R	235	ILE
3	R	238	THR
3	R	242	ILE
3	R	247	ILE

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Mol	Chain	Res	Type
3	R	248	LYS
3	R	250	LEU
3	R	255	VAL
3	R	264	SER
3	R	266	SER
3	R	269	ASP
3	R	272	GLN
3	R	298	GLN
3	R	299	THR
3	R	302	ARG
3	R	307	LYS
3	R	308	PHE
3	R	312	TYR
3	R	313	LEU
3	R	319	ASN
3	R	322	LYS
3	R	323	SER
3	R	345	LEU
3	R	347	ASP
3	R	360	GLU
3	R	364	VAL
3	R	367	ILE
3	R	368	TYR
3	R	373	LEU
3	R	374	LEU
3	R	402	ASN
3	R	410	TYR
3	R	415	LEU
3	R	420	ASP
3	R	429	ARG
3	R	430	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	301	GLN
1	A	656	HIS
2	B	171	HIS
1	D	301	GLN
1	D	656	HIS
1	D	757	GLN
1	G	301	GLN

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Mol	Chain	Res	Type
1	G	656	HIS
1	G	757	GLN
2	H	171	HIS
2	H	389	GLN
1	J	301	GLN
1	J	656	HIS
1	M	301	GLN
1	M	656	HIS
2	N	171	HIS
1	P	301	GLN
1	P	656	HIS
2	Q	171	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 36 ligands modelled in this entry, 6 are monoatomic - leaving 30 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	$\# Z > 2$
4	SO4	A	1001	-	4,4,4	0.27	0	6,6,6	0.22	0
4	SO4	A	1002	-	4,4,4	0.17	0	6,6,6	0.24	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	SO4	A	1003	-	4,4,4	0.18	0	6,6,6	0.18	0
4	SO4	A	1004	-	4,4,4	0.17	0	6,6,6	0.10	0
4	SO4	A	1005	-	4,4,4	0.16	0	6,6,6	0.11	0
4	SO4	D	1001	-	4,4,4	0.27	0	6,6,6	0.21	0
4	SO4	D	1002	-	4,4,4	0.19	0	6,6,6	0.23	0
4	SO4	D	1003	-	4,4,4	0.17	0	6,6,6	0.11	0
4	SO4	D	1004	-	4,4,4	0.14	0	6,6,6	0.11	0
4	SO4	F	601	-	4,4,4	0.16	0	6,6,6	0.10	0
4	SO4	G	901	-	4,4,4	0.17	0	6,6,6	0.24	0
4	SO4	G	902	-	4,4,4	0.17	0	6,6,6	0.16	0
4	SO4	G	903	-	4,4,4	0.15	0	6,6,6	0.11	0
4	SO4	H	1001	-	4,4,4	0.29	0	6,6,6	0.25	0
4	SO4	I	601	-	4,4,4	0.18	0	6,6,6	0.10	0
4	SO4	J	1001	-	4,4,4	0.25	0	6,6,6	0.25	0
4	SO4	J	1002	-	4,4,4	0.17	0	6,6,6	0.17	0
4	SO4	J	1003	-	4,4,4	0.15	0	6,6,6	0.12	0
4	SO4	K	601	-	4,4,4	0.18	0	6,6,6	0.20	0
4	SO4	L	601	-	4,4,4	0.16	0	6,6,6	0.11	0
4	SO4	M	1001	-	4,4,4	0.25	0	6,6,6	0.34	0
4	SO4	M	1002	-	4,4,4	0.18	0	6,6,6	0.20	0
4	SO4	M	1003	-	4,4,4	0.17	0	6,6,6	0.15	0
4	SO4	M	1004	-	4,4,4	0.15	0	6,6,6	0.11	0
4	SO4	O	601	-	4,4,4	0.17	0	6,6,6	0.13	0
4	SO4	P	1001	-	4,4,4	0.27	0	6,6,6	0.32	0
4	SO4	P	1002	-	4,4,4	0.17	0	6,6,6	0.21	0
4	SO4	P	1003	-	4,4,4	0.19	0	6,6,6	0.14	0
4	SO4	P	1004	-	4,4,4	0.17	0	6,6,6	0.14	0
4	SO4	P	1005	-	4,4,4	0.15	0	6,6,6	0.11	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
4	SO4	A	1001	-	-	0/0/0/0	0/0/0/0
4	SO4	A	1002	-	-	0/0/0/0	0/0/0/0
4	SO4	A	1003	-	-	0/0/0/0	0/0/0/0
4	SO4	A	1004	-	-	0/0/0/0	0/0/0/0
4	SO4	A	1005	-	-	0/0/0/0	0/0/0/0
4	SO4	D	1001	-	-	0/0/0/0	0/0/0/0
4	SO4	D	1002	-	-	0/0/0/0	0/0/0/0
4	SO4	D	1003	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	SO4	D	1004	-	-	0/0/0/0	0/0/0/0
4	SO4	F	601	-	-	0/0/0/0	0/0/0/0
4	SO4	G	901	-	-	0/0/0/0	0/0/0/0
4	SO4	G	902	-	-	0/0/0/0	0/0/0/0
4	SO4	G	903	-	-	0/0/0/0	0/0/0/0
4	SO4	H	1001	-	-	0/0/0/0	0/0/0/0
4	SO4	I	601	-	-	0/0/0/0	0/0/0/0
4	SO4	J	1001	-	-	0/0/0/0	0/0/0/0
4	SO4	J	1002	-	-	0/0/0/0	0/0/0/0
4	SO4	J	1003	-	-	0/0/0/0	0/0/0/0
4	SO4	K	601	-	-	0/0/0/0	0/0/0/0
4	SO4	L	601	-	-	0/0/0/0	0/0/0/0
4	SO4	M	1001	-	-	0/0/0/0	0/0/0/0
4	SO4	M	1002	-	-	0/0/0/0	0/0/0/0
4	SO4	M	1003	-	-	0/0/0/0	0/0/0/0
4	SO4	M	1004	-	-	0/0/0/0	0/0/0/0
4	SO4	O	601	-	-	0/0/0/0	0/0/0/0
4	SO4	P	1001	-	-	0/0/0/0	0/0/0/0
4	SO4	P	1002	-	-	0/0/0/0	0/0/0/0
4	SO4	P	1003	-	-	0/0/0/0	0/0/0/0
4	SO4	P	1004	-	-	0/0/0/0	0/0/0/0
4	SO4	P	1005	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1005	SO4	1	0
4	D	1004	SO4	1	0
4	G	903	SO4	1	0
4	J	1003	SO4	1	0
4	M	1004	SO4	1	0
4	P	1005	SO4	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	598/894 (66%)	0.47	60 (10%) 7 4	85, 143, 228, 326	0
1	D	598/894 (66%)	0.51	55 (9%) 9 5	86, 145, 228, 326	0
1	G	598/894 (66%)	0.51	63 (10%) 6 4	83, 145, 229, 339	0
1	J	598/894 (66%)	0.47	52 (8%) 10 6	85, 144, 226, 317	0
1	M	598/894 (66%)	0.50	57 (9%) 8 5	86, 146, 230, 331	0
1	P	598/894 (66%)	0.52	61 (10%) 7 4	86, 144, 230, 328	0
2	B	377/514 (73%)	0.46	20 (5%) 26 14	78, 128, 210, 294	0
2	E	377/514 (73%)	0.43	20 (5%) 26 14	79, 129, 217, 279	0
2	H	377/514 (73%)	0.57	33 (8%) 10 5	79, 128, 210, 283	0
2	K	377/514 (73%)	0.41	26 (6%) 17 9	79, 130, 214, 287	0
2	N	377/514 (73%)	0.53	40 (10%) 6 4	79, 127, 207, 284	0
2	Q	377/514 (73%)	0.52	34 (9%) 9 5	79, 129, 211, 286	0
3	C	303/507 (59%)	0.50	27 (8%) 9 5	82, 158, 242, 312	0
3	F	303/507 (59%)	0.58	28 (9%) 9 5	84, 158, 248, 318	0
3	I	303/507 (59%)	0.53	28 (9%) 9 5	83, 154, 241, 324	0
3	L	303/507 (59%)	0.49	25 (8%) 11 6	83, 160, 241, 326	0
3	O	303/507 (59%)	0.49	30 (9%) 7 4	84, 156, 244, 313	0
3	R	303/507 (59%)	0.45	28 (9%) 9 5	83, 155, 242, 334	0
All	All	7668/11490 (66%)	0.50	687 (8%) 9 5	78, 141, 230, 339	0

All (687) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	I	324	MET	16.6
1	M	532	GLU	11.2
1	D	196	TYR	10.3

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Mol	Chain	Res	Type	RSRZ
3	I	369	ALA	9.7
3	L	424	PHE	9.2
3	C	369	ALA	8.7
1	A	261	VAL	8.3
3	F	347	ASP	8.0
1	P	651	SER	8.0
1	P	182	LEU	8.0
1	A	651	SER	7.9
3	R	424	PHE	7.9
1	P	261	VAL	7.8
1	A	304	ASP	7.2
1	D	261	VAL	6.5
2	Q	156	LEU	6.5
1	A	247	ILE	6.5
1	D	247	ILE	6.4
3	L	137	SER	6.3
3	O	369	ALA	6.2
1	M	196	TYR	6.2
1	A	262	GLY	6.2
1	M	247	ILE	6.2
1	G	532	GLU	6.1
1	J	182	LEU	6.0
1	J	237	GLU	5.9
3	O	324	MET	5.9
1	D	532	GLU	5.9
2	N	156	LEU	5.9
1	J	532	GLU	5.9
3	F	143	THR	5.8
3	L	408	ILE	5.7
2	B	294	HIS	5.6
3	I	370	SER	5.6
3	I	428	SER	5.6
1	G	245	ILE	5.5
3	C	370	SER	5.4
1	D	304	ASP	5.4
1	P	496	THR	5.3
3	O	347	ASP	5.3
1	D	305	PHE	5.3
2	B	129	PHE	5.2
3	C	411	VAL	5.2
1	A	205	TYR	5.1
2	N	225	GLN	5.1

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Mol	Chain	Res	Type	RSRZ
1	D	654	LEU	5.0
1	P	456	VAL	5.0
3	C	245	VAL	4.9
3	C	318	ILE	4.9
2	E	129	PHE	4.9
2	H	318	LEU	4.9
3	F	411	VAL	4.9
1	M	698	LYS	4.9
3	R	365	TRP	4.9
2	H	156	LEU	4.8
1	A	225	LEU	4.8
1	A	305	PHE	4.8
1	G	196	TYR	4.8
3	F	245	VAL	4.8
1	J	216	ILE	4.8
3	F	369	ALA	4.8
2	Q	184	TRP	4.7
1	D	683	PHE	4.7
1	J	456	VAL	4.7
1	D	262	GLY	4.6
3	F	370	SER	4.6
1	D	185	GLN	4.6
2	K	327	PRO	4.6
2	H	294	HIS	4.6
2	Q	482	HIS	4.6
3	F	373	LEU	4.5
1	D	455	LYS	4.4
3	F	408	ILE	4.4
2	Q	318	LEU	4.4
1	M	456	VAL	4.4
3	O	372	HIS	4.4
1	G	329	ILE	4.4
1	M	455	LYS	4.4
2	N	327	PRO	4.4
1	G	574	TRP	4.3
1	P	260	LEU	4.3
1	P	304	ASP	4.3
1	G	698	LYS	4.3
1	J	457	LYS	4.3
3	R	368	TYR	4.3
1	P	532	GLU	4.3
1	P	217	ALA	4.3

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Mol	Chain	Res	Type	RSRZ
1	A	489	PHE	4.2
1	G	683	PHE	4.2
1	M	182	LEU	4.2
1	P	768	TYR	4.1
1	J	748	GLU	4.1
1	J	462	ILE	4.1
1	P	218	VAL	4.1
1	M	225	LEU	4.1
2	N	136	ILE	4.1
3	F	365	TRP	4.1
1	D	237	GLU	4.1
1	J	261	VAL	4.0
1	G	272	PHE	4.0
1	M	539	VAL	4.0
1	M	285	MET	4.0
1	G	651	SER	4.0
2	Q	294	HIS	4.0
2	K	94	LYS	4.0
1	G	247	ILE	4.0
2	Q	326	TYR	4.0
1	P	245	ILE	4.0
1	D	476	ILE	4.0
1	P	205	TYR	3.9
2	N	417	PHE	3.9
1	M	274	ILE	3.9
2	H	115	GLN	3.9
3	R	369	ALA	3.9
3	L	368	TYR	3.9
3	L	411	VAL	3.9
1	A	185	GLN	3.9
3	I	372	HIS	3.9
3	O	374	LEU	3.9
1	P	329	ILE	3.9
1	D	699	LEU	3.9
1	M	219	LEU	3.8
1	P	462	ILE	3.8
2	N	476	ILE	3.8
3	O	373	LEU	3.8
1	P	262	GLY	3.8
3	C	373	LEU	3.8
1	J	217	ALA	3.8
1	G	274	ILE	3.8

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Mol	Chain	Res	Type	RSRZ
1	M	654	LEU	3.8
3	C	347	ASP	3.8
3	O	376	ALA	3.8
1	P	237	GLU	3.8
1	P	214	LEU	3.8
1	G	198	ASP	3.7
2	Q	198	ILE	3.7
1	D	263	ILE	3.7
1	D	281	SER	3.7
1	M	276	SER	3.7
3	R	374	LEU	3.7
1	M	284	VAL	3.7
1	A	50	LEU	3.7
3	O	370	SER	3.7
1	A	747	LEU	3.7
2	E	118	TRP	3.7
3	R	422	GLY	3.6
1	P	422	ILE	3.6
1	G	182	LEU	3.6
1	A	272	PHE	3.6
3	F	376	ALA	3.6
1	J	654	LEU	3.6
1	P	711	LEU	3.6
2	N	491	PHE	3.6
1	D	651	SER	3.6
1	M	304	ASP	3.6
3	L	415	LEU	3.6
1	A	245	ILE	3.6
2	N	115	GLN	3.5
1	G	496	THR	3.5
2	K	295	THR	3.5
1	J	465	VAL	3.5
1	G	304	ASP	3.5
1	D	205	TYR	3.5
2	N	129	PHE	3.5
3	F	424	PHE	3.5
1	J	196	TYR	3.5
1	M	329	ILE	3.5
1	M	183	ASP	3.5
1	M	184	SER	3.5
2	K	219	ILE	3.5
3	R	428	SER	3.5

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Mol	Chain	Res	Type	RSRZ
1	G	539	VAL	3.5
1	D	271	ILE	3.5
1	A	683	PHE	3.5
2	N	318	LEU	3.5
1	A	478	MET	3.5
1	M	548	TYR	3.4
1	P	550	TYR	3.4
2	Q	125	PHE	3.4
1	M	699	LEU	3.4
1	P	533	LEU	3.4
2	K	318	LEU	3.4
1	A	182	LEU	3.4
3	I	374	LEU	3.4
1	A	236	ILE	3.4
1	M	275	GLU	3.4
1	D	748	GLU	3.4
3	O	320	CYS	3.4
1	J	304	ASP	3.4
1	M	580	ASN	3.4
2	Q	129	PHE	3.4
3	C	376	ALA	3.3
3	C	372	HIS	3.3
2	H	491	PHE	3.3
1	P	305	PHE	3.3
3	R	27	ILE	3.3
1	D	198	ASP	3.3
1	A	550	TYR	3.3
3	R	415	LEU	3.3
2	N	309	TYR	3.3
1	J	547	VAL	3.3
1	M	289	SER	3.3
1	D	236	ILE	3.2
3	L	365	TRP	3.2
2	E	513	MET	3.2
2	H	367	PHE	3.2
1	D	478	MET	3.2
2	K	125	PHE	3.2
1	P	225	LEU	3.2
2	N	330	TRP	3.2
1	A	630	LEU	3.2
2	N	131	HIS	3.2
1	J	242	ILE	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	316	ALA	3.2
1	D	62	LYS	3.2
3	I	367	ILE	3.2
3	F	317	LEU	3.2
1	A	237	GLU	3.1
2	E	136	ILE	3.1
1	A	654	LEU	3.1
1	D	489	PHE	3.1
3	I	371	CYS	3.1
3	L	270	PHE	3.1
1	M	574	TRP	3.1
2	K	322	ARG	3.1
1	D	626	LEU	3.1
1	A	422	ILE	3.1
2	H	476	ILE	3.1
1	M	611	ILE	3.1
3	I	421	LYS	3.1
3	R	137	SER	3.1
2	Q	322	ARG	3.1
1	A	660	LYS	3.1
1	J	496	THR	3.1
2	Q	295	THR	3.1
3	C	365	TRP	3.1
1	A	672	ILE	3.1
3	R	270	PHE	3.1
1	D	284	VAL	3.1
1	P	749	LYS	3.1
2	N	311	MET	3.1
2	H	111	ILE	3.1
1	A	233	VAL	3.1
1	D	227	LEU	3.1
1	G	184	SER	3.0
1	G	284	VAL	3.0
1	M	245	ILE	3.0
2	Q	115	GLN	3.0
2	H	472	ARG	3.0
3	C	324	MET	3.0
3	O	371	CYS	3.0
1	D	461	HIS	3.0
1	D	533	LEU	3.0
1	P	714	PHE	3.0
3	L	349	ILE	3.0

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Mol	Chain	Res	Type	RSRZ
2	Q	208	PRO	3.0
2	B	318	LEU	3.0
1	M	468	VAL	3.0
1	P	65	LEU	3.0
2	Q	249	CYS	3.0
1	A	317	ILE	3.0
1	G	246	LYS	3.0
1	A	495	SER	3.0
1	P	216	ILE	3.0
1	P	495	SER	3.0
1	A	499	GLU	3.0
2	E	104	PHE	3.0
1	A	263	ILE	3.0
1	A	704	LEU	3.0
1	J	219	LEU	3.0
1	M	214	LEU	3.0
1	M	533	LEU	3.0
1	P	465	VAL	3.0
2	E	287	TRP	2.9
1	D	711	LEU	2.9
1	D	245	ILE	2.9
1	J	422	ILE	2.9
1	A	574	TRP	2.9
2	H	157	HIS	2.9
2	N	480	LEU	2.9
3	C	317	LEU	2.9
1	J	461	HIS	2.9
2	H	198	ILE	2.9
3	L	370	SER	2.9
1	G	623	LEU	2.9
2	H	343	THR	2.9
1	J	58	HIS	2.9
1	P	184	SER	2.9
1	J	752	LEU	2.9
2	N	176	VAL	2.9
2	Q	192	TYR	2.9
2	N	126	PRO	2.9
2	H	162	ILE	2.9
2	H	314	ILE	2.9
1	M	272	PHE	2.9
3	L	363	GLU	2.9
2	K	129	PHE	2.9

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Mol	Chain	Res	Type	RSRZ
3	C	421	LYS	2.9
2	K	208	PRO	2.9
1	J	589	ILE	2.8
2	Q	367	PHE	2.8
1	D	187	ILE	2.8
1	M	237	GLU	2.8
3	I	21	TYR	2.8
1	G	725	VAL	2.8
3	F	27	ILE	2.8
2	B	184	TRP	2.8
1	G	233	VAL	2.8
1	M	462	ILE	2.8
1	D	316	ALA	2.8
2	Q	211	TYR	2.8
3	C	278	TYR	2.8
1	M	476	ILE	2.8
1	P	685	TYR	2.8
2	N	159	THR	2.8
3	I	368	TYR	2.8
3	I	416	LYS	2.8
3	R	222	LEU	2.8
1	P	457	LYS	2.8
2	H	327	PRO	2.8
2	E	309	TYR	2.8
3	L	369	ALA	2.8
3	C	408	ILE	2.8
1	G	567	ILE	2.8
2	H	137	TRP	2.8
2	B	287	TRP	2.7
1	P	204	ALA	2.7
1	D	434	ARG	2.7
1	G	550	TYR	2.7
3	O	137	SER	2.7
1	A	568	ILE	2.7
1	P	274	ILE	2.7
2	N	109	GLN	2.7
3	I	320	CYS	2.7
1	P	227	LEU	2.7
3	O	411	VAL	2.7
3	R	411	VAL	2.7
1	G	434	ARG	2.7
2	K	136	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
2	Q	215	LEU	2.7
2	E	317	MET	2.7
1	P	383	ILE	2.7
1	A	699	LEU	2.7
1	D	184	SER	2.7
1	J	463	LEU	2.7
1	J	272	PHE	2.7
2	K	330	TRP	2.7
3	C	314	TRP	2.7
1	A	509	GLU	2.7
3	C	368	TYR	2.7
1	M	246	LYS	2.7
2	N	197	GLU	2.7
1	J	271	ILE	2.7
3	O	317	LEU	2.7
2	Q	478	ARG	2.7
1	J	651	SER	2.7
1	M	496	THR	2.7
1	J	550	TYR	2.6
1	P	181	ARG	2.6
3	I	27	ILE	2.6
3	O	235	ILE	2.6
2	K	184	TRP	2.6
1	J	225	LEU	2.6
3	L	374	LEU	2.6
1	D	630	LEU	2.6
1	P	187	ILE	2.6
2	N	219	ILE	2.6
3	I	439	GLU	2.6
3	I	317	LEU	2.6
1	G	549	TYR	2.6
1	M	457	LYS	2.6
2	B	509	CYS	2.6
2	K	482	HIS	2.6
1	G	699	LEU	2.6
2	B	215	LEU	2.6
1	D	762	ARG	2.6
1	D	552	LEU	2.6
3	C	27	ILE	2.6
1	P	263	ILE	2.6
2	E	502	ILE	2.6
3	I	434	GLN	2.6

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Mol	Chain	Res	Type	RSRZ
3	F	195	LEU	2.6
3	L	297	PHE	2.6
1	G	225	LEU	2.6
2	E	311	MET	2.6
2	Q	479	LEU	2.6
3	I	274	MET	2.6
1	M	202	ILE	2.6
1	D	499	GLU	2.6
2	K	341	ARG	2.6
1	D	422	ILE	2.6
1	D	511	ILE	2.6
1	M	305	PHE	2.5
1	A	469	TYR	2.5
1	A	227	LEU	2.5
1	A	538	LEU	2.5
1	A	467	PHE	2.5
1	J	538	LEU	2.5
1	D	672	ILE	2.5
2	N	314	ILE	2.5
1	A	58	HIS	2.5
2	Q	181	TYR	2.5
2	B	135	ILE	2.5
2	B	182	ILE	2.5
2	H	116	ILE	2.5
1	P	250	ALA	2.5
2	N	177	TYR	2.5
1	G	732	LEU	2.5
2	K	226	LEU	2.5
2	Q	222	PHE	2.5
3	R	431	ILE	2.5
2	Q	264	PRO	2.5
2	K	215	LEU	2.5
3	O	346	ILE	2.5
3	R	140	ILE	2.5
1	G	748	GLU	2.5
2	H	309	TYR	2.5
1	A	679	LEU	2.5
3	R	216	LEU	2.5
2	N	111	ILE	2.5
3	F	199	LYS	2.5
3	I	436	LYS	2.5
1	G	456	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
2	Q	491	PHE	2.5
3	I	19	LEU	2.5
1	P	578	PHE	2.5
2	Q	108	PHE	2.5
1	A	482	SER	2.5
2	B	118	TRP	2.5
1	A	196	TYR	2.5
2	N	168	ALA	2.5
1	D	272	PHE	2.5
1	A	476	ILE	2.5
1	D	233	VAL	2.4
1	M	300	LEU	2.4
2	N	192	TYR	2.4
1	A	420	GLU	2.4
1	D	462	ILE	2.4
3	C	24	ILE	2.4
1	M	427	SER	2.4
3	O	428	SER	2.4
1	A	711	LEU	2.4
1	P	702	LEU	2.4
2	E	192	TYR	2.4
2	Q	502	ILE	2.4
1	J	184	SER	2.4
2	N	175	PRO	2.4
2	B	235	GLY	2.4
3	C	227	HIS	2.4
3	F	227	HIS	2.4
1	J	185	GLN	2.4
3	R	408	ILE	2.4
2	B	123	MET	2.4
1	D	225	LEU	2.4
1	J	218	VAL	2.4
3	C	253	ILE	2.4
3	L	81	GLU	2.4
1	A	214	LEU	2.4
3	F	270	PHE	2.4
1	G	402	ILE	2.4
2	N	162	ILE	2.4
3	L	86	SER	2.4
1	G	214	LEU	2.4
3	C	374	LEU	2.4
3	I	231	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
2	B	309	TYR	2.4
1	P	183	ASP	2.4
1	G	261	VAL	2.4
3	O	421	LYS	2.4
1	G	380	MET	2.4
3	L	274	MET	2.4
1	G	330	PRO	2.4
1	G	682	PHE	2.4
1	J	495	SER	2.4
1	M	549	TYR	2.4
1	G	58	HIS	2.4
3	O	222	LEU	2.4
1	G	509	GLU	2.4
1	M	759	GLU	2.4
2	K	192	TYR	2.4
2	K	326	TYR	2.4
2	N	181	TYR	2.4
1	G	611	ILE	2.3
1	J	204	ALA	2.3
3	L	23	TYR	2.3
2	K	156	LEU	2.3
1	M	58	HIS	2.3
3	O	270	PHE	2.3
1	J	549	TYR	2.3
2	E	318	LEU	2.3
1	G	495	SER	2.3
2	K	502	ILE	2.3
3	O	323	SER	2.3
1	P	272	PHE	2.3
2	Q	452	PHE	2.3
3	R	2	PHE	2.3
3	R	423	GLY	2.3
2	K	115	GLN	2.3
1	J	65	LEU	2.3
1	J	552	LEU	2.3
1	A	708	VAL	2.3
3	F	144	VAL	2.3
3	L	428	SER	2.3
1	G	219	LEU	2.3
1	G	672	ILE	2.3
3	F	368	TYR	2.3
1	D	482	SER	2.3

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Mol	Chain	Res	Type	RSRZ
3	F	138	PHE	2.3
2	E	156	LEU	2.3
3	F	2	PHE	2.3
1	D	397	LYS	2.3
3	R	274	MET	2.3
1	P	58	HIS	2.3
1	A	508	ILE	2.3
2	H	152	LEU	2.3
1	J	205	TYR	2.3
2	K	182	ILE	2.3
2	Q	164	ILE	2.3
1	D	747	LEU	2.3
3	C	415	LEU	2.3
1	A	286	VAL	2.3
1	M	550	TYR	2.3
3	R	152	ILE	2.3
3	L	138	PHE	2.3
1	M	621	LYS	2.3
1	J	719	LEU	2.3
2	N	152	LEU	2.3
3	I	239	LEU	2.3
1	A	301	GLN	2.3
1	P	247	ILE	2.3
3	C	87	VAL	2.3
1	G	457	LYS	2.3
3	F	198	LEU	2.3
2	E	330	TRP	2.3
3	I	376	ALA	2.3
3	I	411	VAL	2.3
3	L	208	TYR	2.3
2	N	343	THR	2.3
3	I	349	ILE	2.3
1	M	623	LEU	2.2
2	E	215	LEU	2.2
1	G	476	ILE	2.2
3	L	140	ILE	2.2
2	H	446	TYR	2.2
2	Q	330	TRP	2.2
2	B	282	ARG	2.2
3	F	211	ARG	2.2
1	G	187	ILE	2.2
2	H	287	TRP	2.2

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Mol	Chain	Res	Type	RSRZ
1	G	372	ILE	2.2
1	M	725	VAL	2.2
3	F	412	ARG	2.2
3	O	434	GLN	2.2
1	M	538	LEU	2.2
1	D	216	ILE	2.2
1	J	263	ILE	2.2
1	M	216	ILE	2.2
2	B	136	ILE	2.2
2	H	331	ILE	2.2
1	A	619	GLU	2.2
2	H	159	THR	2.2
1	G	747	LEU	2.2
1	P	479	HIS	2.2
3	I	304	HIS	2.2
3	C	305	THR	2.2
3	O	143	THR	2.2
1	J	578	PHE	2.2
1	M	371	LYS	2.2
1	P	547	VAL	2.2
2	B	502	ILE	2.2
1	P	206	ALA	2.2
1	J	554	ASN	2.2
1	J	574	TRP	2.2
2	B	491	PHE	2.2
3	O	425	ALA	2.2
2	H	374	THR	2.2
1	P	748	GLU	2.2
3	F	28	SER	2.2
1	A	434	ARG	2.2
3	O	19	LEU	2.2
1	G	489	PHE	2.2
2	E	135	ILE	2.2
2	H	311	MET	2.2
2	Q	96	ILE	2.2
2	N	307	LEU	2.2
1	M	444	PRO	2.2
1	A	187	ILE	2.2
2	N	116	ILE	2.2
2	Q	335	THR	2.2
3	L	183	GLU	2.2
1	P	502	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	J	533	LEU	2.2
2	K	338	LEU	2.2
1	J	467	PHE	2.2
1	P	589	ILE	2.2
2	K	352	ILE	2.2
3	I	318	ILE	2.2
1	D	679	LEU	2.1
1	A	184	SER	2.1
1	G	183	ASP	2.1
1	P	611	ILE	2.1
2	H	176	VAL	2.1
3	R	4	VAL	2.1
1	M	449	LEU	2.1
1	P	574	TRP	2.1
2	N	226	LEU	2.1
1	P	537	PHE	2.1
2	H	129	PHE	2.1
1	P	740	ILE	2.1
2	H	378	LEU	2.1
3	O	345	LEU	2.1
1	G	417	THR	2.1
1	P	177	THR	2.1
1	A	755	PRO	2.1
1	G	276	SER	2.1
2	H	175	PRO	2.1
2	H	487	LEU	2.1
2	E	294	HIS	2.1
3	C	416	LYS	2.1
3	R	226	ARG	2.1
1	J	383	ILE	2.1
1	M	752	LEU	2.1
3	R	86	SER	2.1
3	R	23	TYR	2.1
1	D	169	GLN	2.1
2	K	331	ILE	2.1
1	G	729	ALA	2.1
1	A	748	GLU	2.1
1	M	704	LEU	2.1
3	L	226	ARG	2.1
3	O	231	LEU	2.1
1	G	244	SER	2.1
3	F	137	SER	2.1

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Mol	Chain	Res	Type	RSRZ
3	F	428	SER	2.1
1	G	237	GLU	2.1
1	P	284	VAL	2.1
2	H	131	HIS	2.1
2	K	314	ILE	2.1
1	M	434	ARG	2.1
1	J	398	ALA	2.1
1	A	399	TRP	2.1
1	J	483	HIS	2.1
2	E	354	LYS	2.1
2	B	156	LEU	2.1
1	G	250	ALA	2.1
1	G	621	LYS	2.1
1	G	422	ILE	2.1
2	Q	314	ILE	2.1
3	F	87	VAL	2.1
1	P	219	LEU	2.1
2	Q	276	PHE	2.1
3	C	23	TYR	2.1
1	G	242	ILE	2.1
1	J	203	ILE	2.1
2	N	140	ILE	2.1
2	H	282	ARG	2.1
2	N	164	ILE	2.1
2	Q	219	ILE	2.1
3	R	370	SER	2.1
3	R	209	ARG	2.0
1	D	50	LEU	2.0
1	G	263	ILE	2.0
2	N	137	TRP	2.0
1	A	511	ILE	2.0
1	G	442	LEU	2.0
1	G	538	LEU	2.0
1	P	264	ILE	2.0
3	I	305	THR	2.0
1	G	289	SER	2.0
1	D	317	ILE	2.0
1	J	243	LYS	2.0
2	B	164	ILE	2.0
2	E	102	LEU	2.0
3	O	256	GLU	2.0
3	R	81	GLU	2.0

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Mol	Chain	Res	Type	RSRZ
1	J	284	VAL	2.0
1	M	303	VAL	2.0
2	N	489	VAL	2.0
3	O	368	TYR	2.0
2	B	300	ASN	2.0
3	L	418	CYS	2.0
2	H	259	GLN	2.0
2	E	306	VAL	2.0
3	O	33	ARG	2.0
2	N	125	PHE	2.0
2	N	229	LYS	2.0
3	O	219	LEU	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. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	MG	P	1006	1/1	0.23	0.28	108,108,108,108	0
4	SO4	D	1004	5/5	0.33	0.58	172,284,325,366	0
4	SO4	M	1004	5/5	0.36	0.38	164,293,328,365	0
4	SO4	A	1005	5/5	0.39	0.46	161,270,297,338	0
5	MG	J	1004	1/1	0.53	0.26	106,106,106,106	0
4	SO4	J	1003	5/5	0.57	0.26	166,284,321,362	0
4	SO4	G	903	5/5	0.62	0.23	164,281,309,354	0
5	MG	A	1006	1/1	0.67	0.23	107,107,107,107	0
4	SO4	M	1002	5/5	0.69	0.27	169,171,179,191	0
4	SO4	P	1005	5/5	0.71	0.18	166,296,344,363	0
4	SO4	O	601	5/5	0.77	0.24	101,215,246,246	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	SO4	P	1002	5/5	0.80	0.30	166,168,172,186	0
5	MG	G	904	1/1	0.81	0.34	108,108,108,108	0
5	MG	D	1005	1/1	0.84	0.17	107,107,107,107	0
4	SO4	I	601	5/5	0.86	0.22	98,191,239,244	0
4	SO4	A	1003	5/5	0.86	0.15	98,142,149,150	0
4	SO4	K	601	5/5	0.86	0.20	165,172,176,184	0
5	MG	M	1005	1/1	0.87	0.32	108,108,108,108	0
4	SO4	G	902	5/5	0.87	0.15	117,133,146,149	0
4	SO4	A	1002	5/5	0.87	0.21	163,169,175,184	0
4	SO4	G	901	5/5	0.88	0.34	153,155,162,180	0
4	SO4	D	1002	5/5	0.88	0.18	144,165,173,183	0
4	SO4	P	1003	5/5	0.88	0.17	111,150,158,158	0
4	SO4	L	601	5/5	0.89	0.22	101,201,236,237	0
4	SO4	F	601	5/5	0.89	0.22	99,179,235,237	0
4	SO4	J	1002	5/5	0.91	0.16	106,127,143,149	0
4	SO4	A	1004	5/5	0.91	0.30	95,186,233,252	0
4	SO4	D	1003	5/5	0.92	0.17	104,134,141,147	0
4	SO4	P	1004	5/5	0.92	0.27	96,187,207,226	0
4	SO4	A	1001	5/5	0.93	0.22	96,110,115,123	0
4	SO4	D	1001	5/5	0.94	0.19	94,106,110,111	0
4	SO4	M	1001	5/5	0.94	0.28	92,110,119,130	0
4	SO4	M	1003	5/5	0.96	0.14	107,162,234,240	0
4	SO4	P	1001	5/5	0.96	0.19	94,105,113,126	0
4	SO4	H	1001	5/5	0.97	0.25	92,92,108,112	0
4	SO4	J	1001	5/5	0.98	0.18	94,108,113,120	0

6.5 Other polymers

There are no such residues in this entry.