



Full wwPDB X-ray Structure Validation Report ⓘ

Jul 31, 2017 – 05:03 PM EDT

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 : unknown
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

<http://wwpdb.org/validation/2016/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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20029824
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20029824

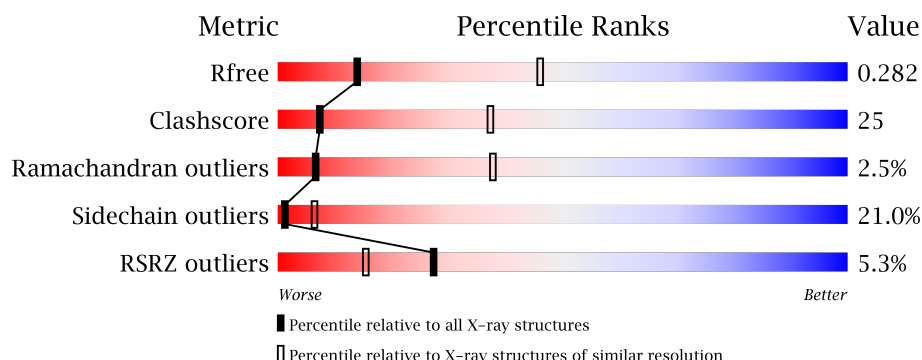
1 Overall quality at a glance

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.



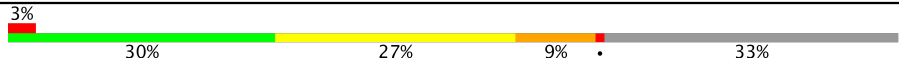
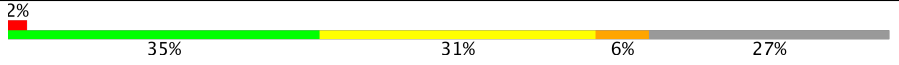
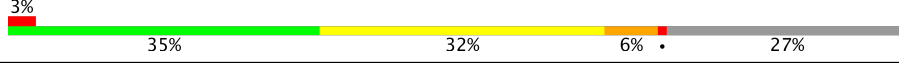
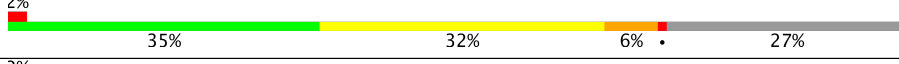
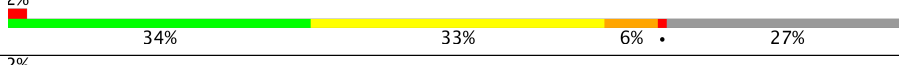
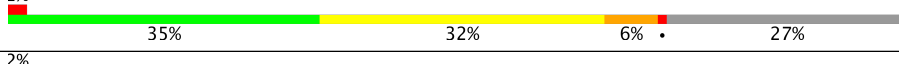
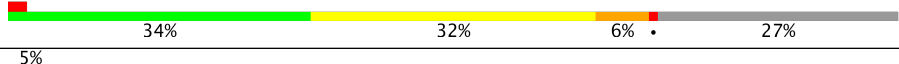
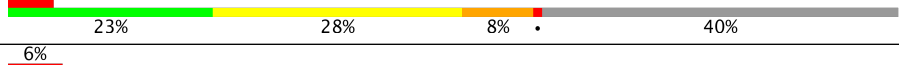





Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	1015 (3.22-3.18)
Clashscore	112137	1009 (3.20-3.20)
Ramachandran outliers	110173	1118 (3.22-3.18)
Sidechain outliers	110143	1117 (3.22-3.18)
RSRZ outliers	101464	1020 (3.22-3.18)

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>4%</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>3%</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>3%</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>3%</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>3%</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
1	P	894	
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	1001	-	-	-	X
4	SO4	A	1004	-	-	-	X
4	SO4	D	1001	-	-	-	X
4	SO4	D	1002	-	-	-	X
4	SO4	F	601	-	-	-	X
4	SO4	G	901	-	-	-	X
4	SO4	H	1001	-	-	-	X
4	SO4	I	601	-	-	-	X
4	SO4	J	1001	-	-	-	X
4	SO4	K	601	-	-	-	X
4	SO4	L	601	-	-	-	X
4	SO4	M	1001	-	-	-	X
4	SO4	M	1002	-	-	-	X
4	SO4	O	601	-	-	-	X
4	SO4	P	1001	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	SO4	P	1002	-	-	-	X
4	SO4	P	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			

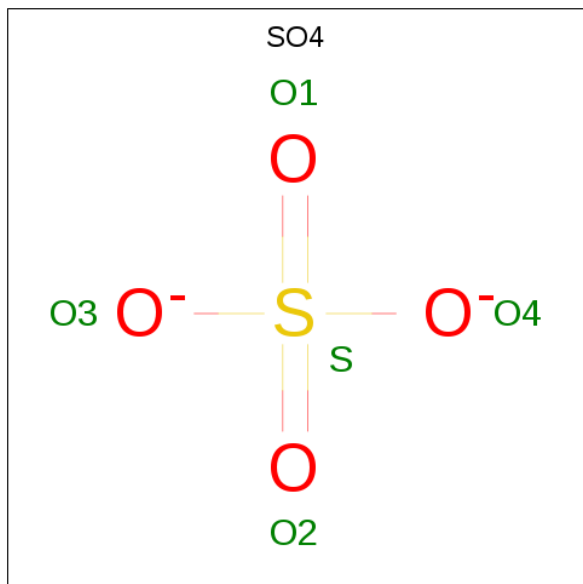
- Molecule 2 is a protein called RNA polymerase I-specific transcription initiation factor RRN7.

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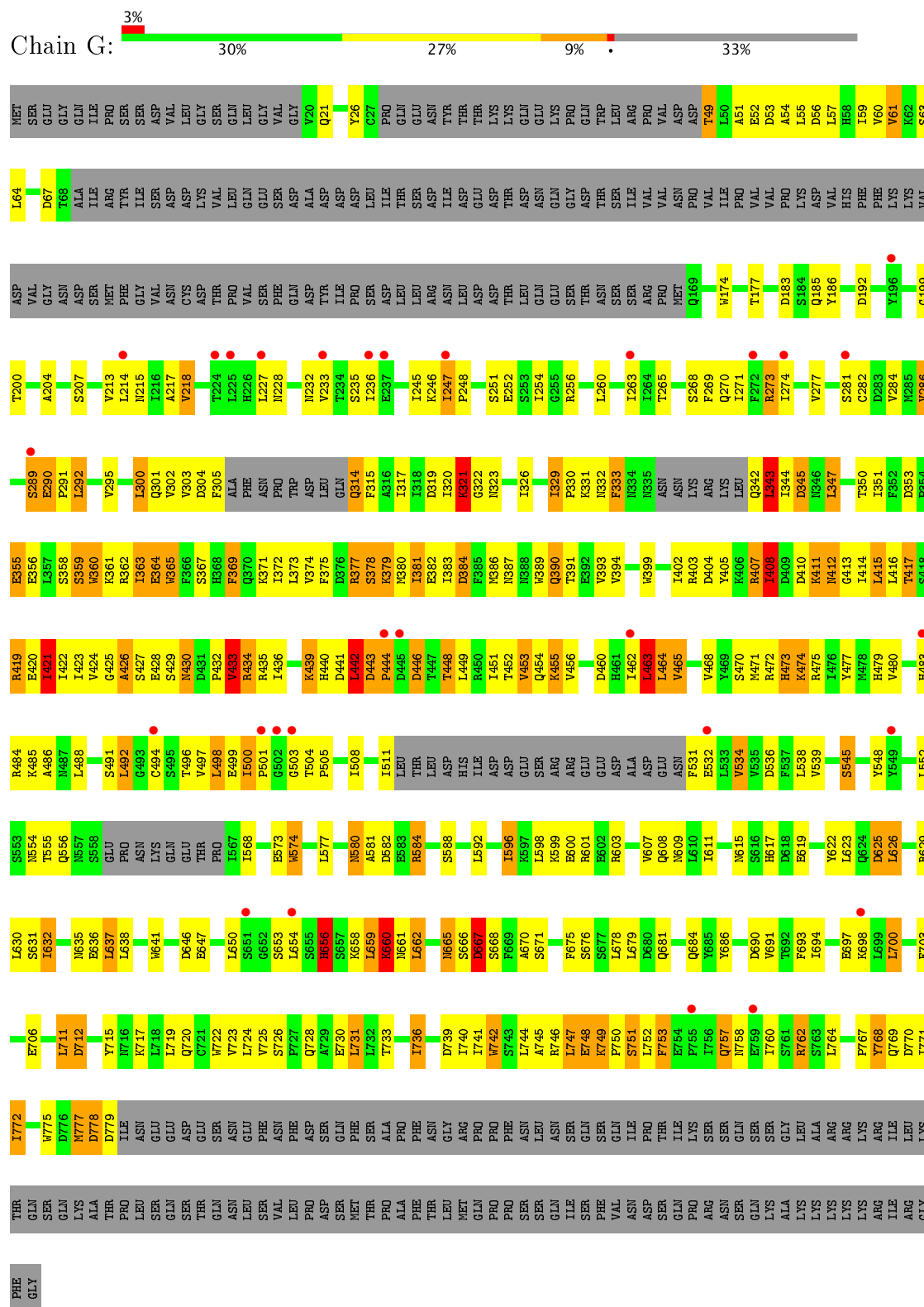
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	P	1	Total	O	S	0	0
			5	4	1		
4	P	1	Total	O	S	0	0
			5	4	1		
4	P	1	Total	O	S	0	0
			5	4	1		

- 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		

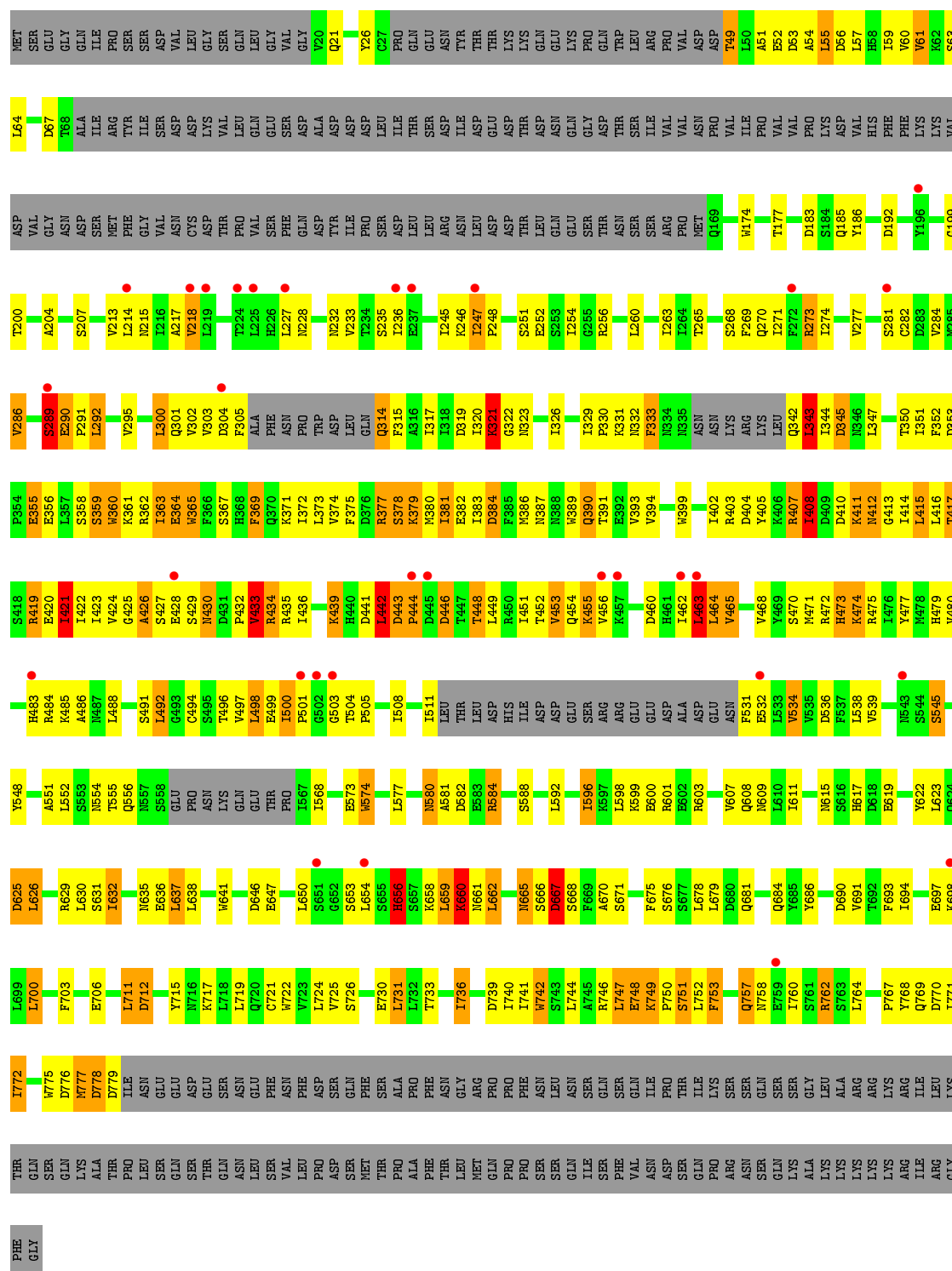


- Molecule 1: RNA polymerase I-specific transcription initiation factor RRN6

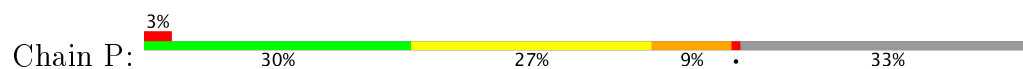


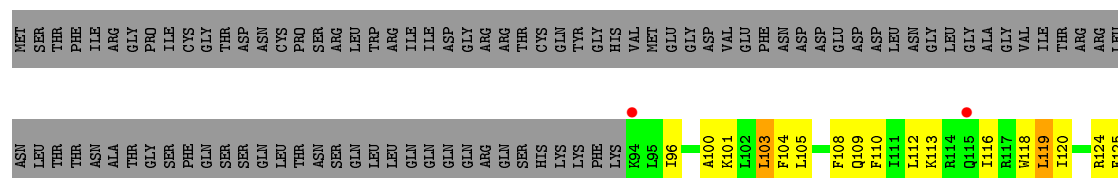
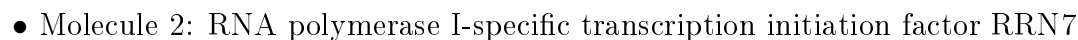
- Molecule 1: RNA polymerase I-specific transcription initiation factor RRN6

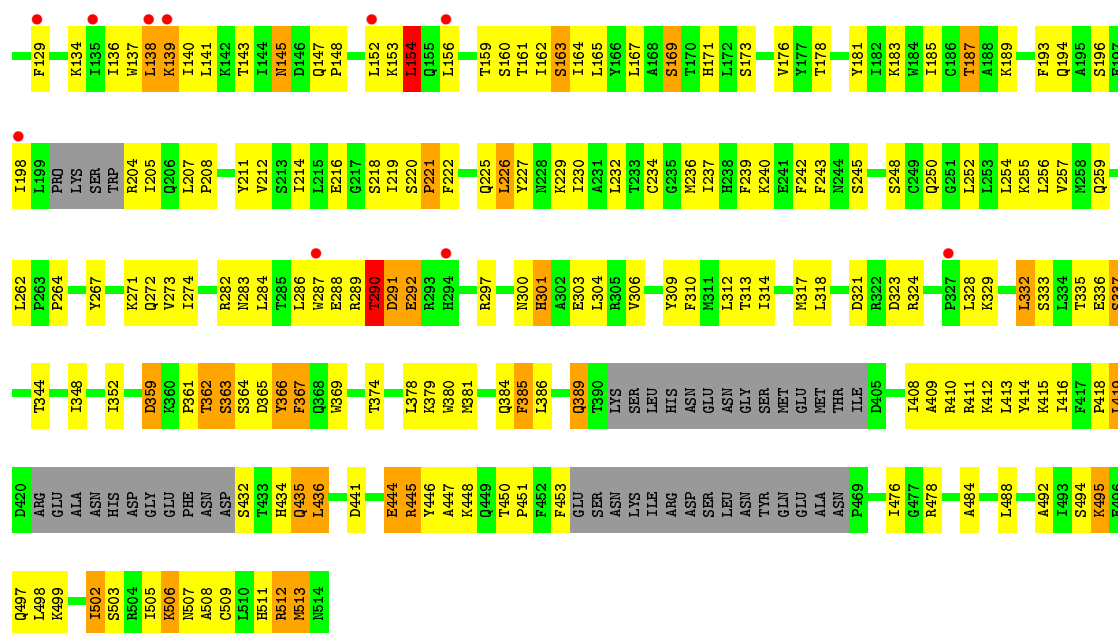




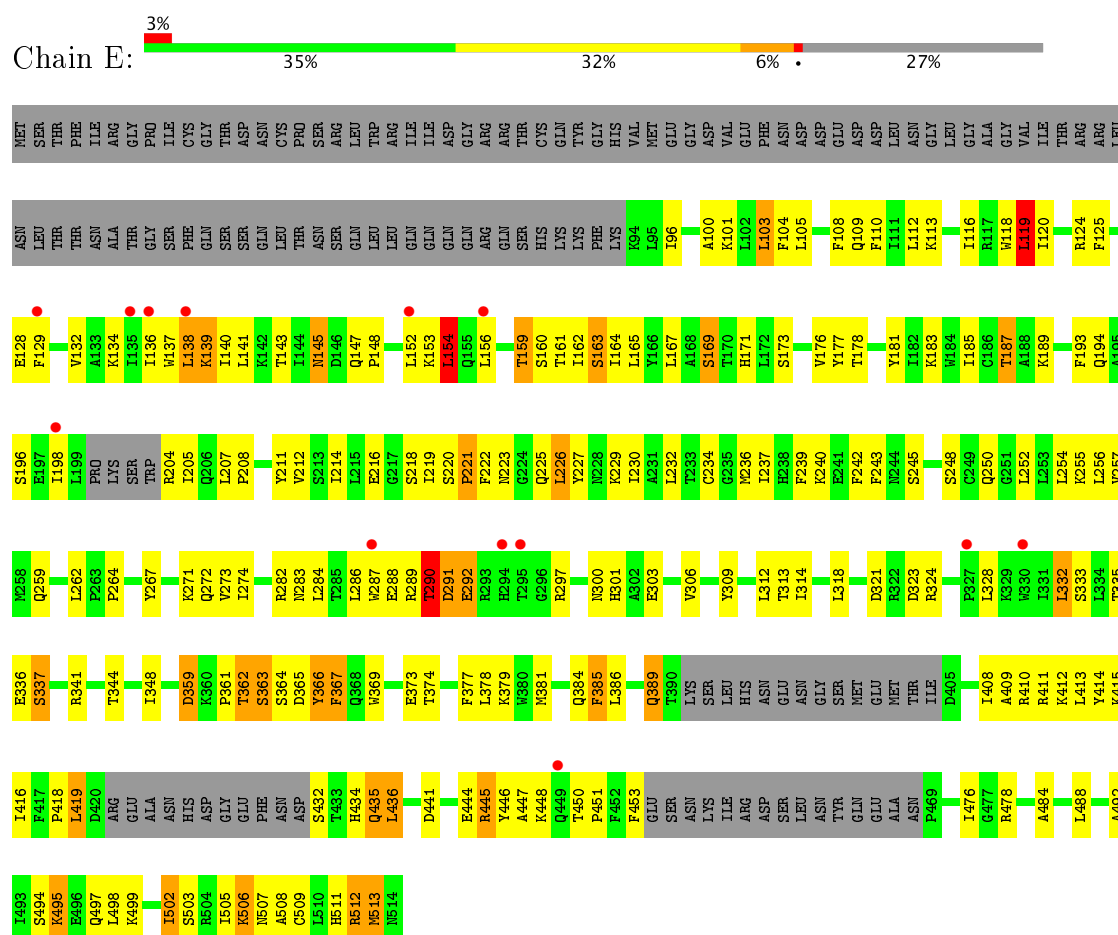
• Molecule 1: RNA polymerase I-specific transcription initiation factor RRN6





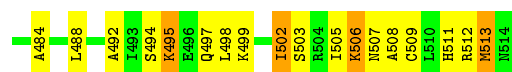


• Molecule 2: RNA polymerase I-specific transcription initiation factor RRN7

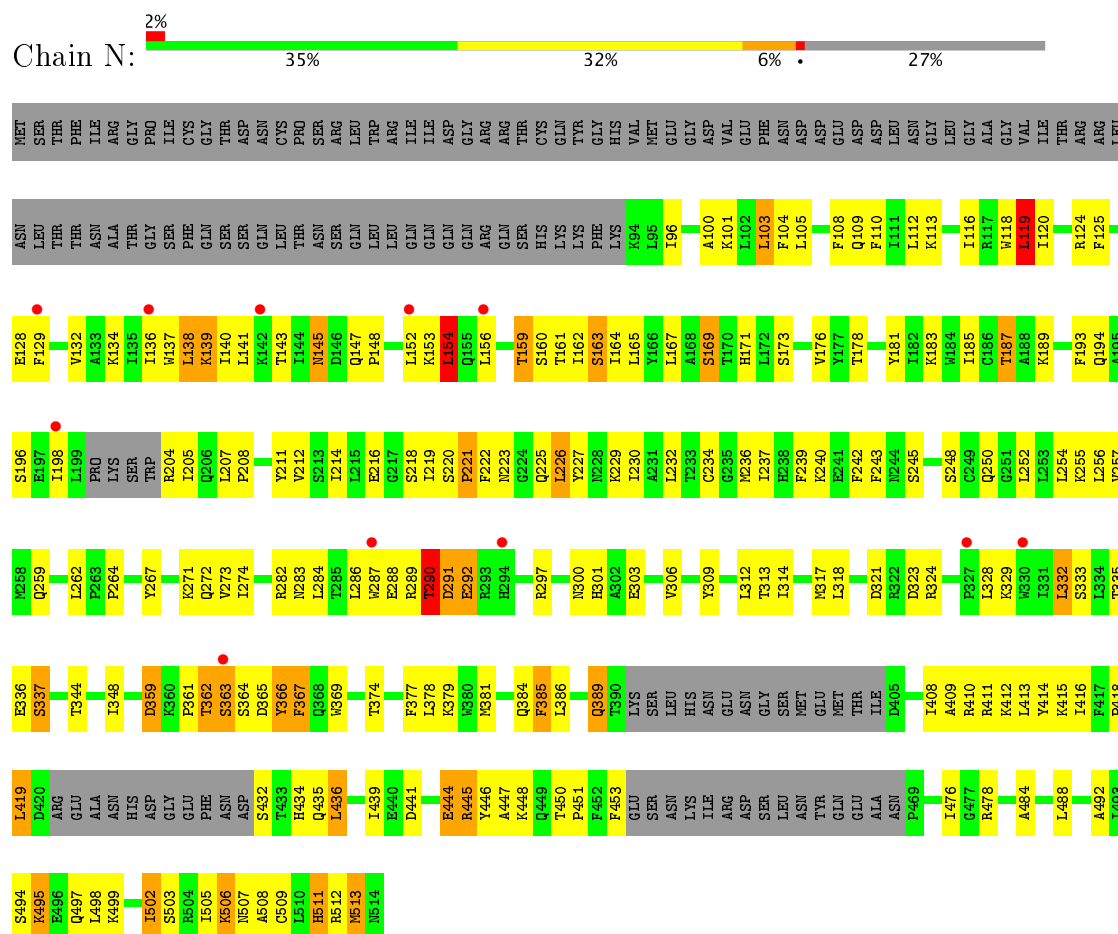


• Molecule 2: RNA polymerase I-specific transcription initiation factor RRN7

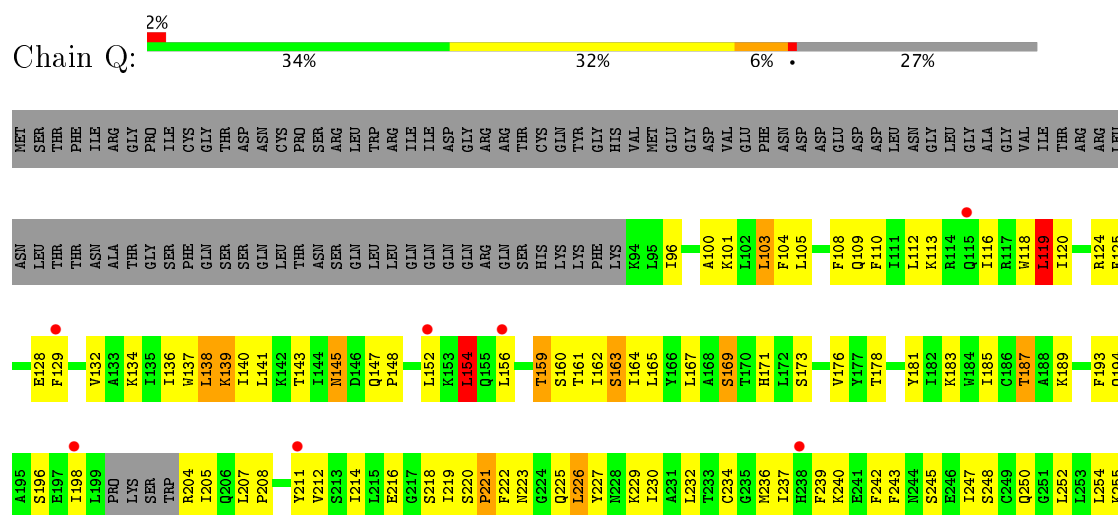


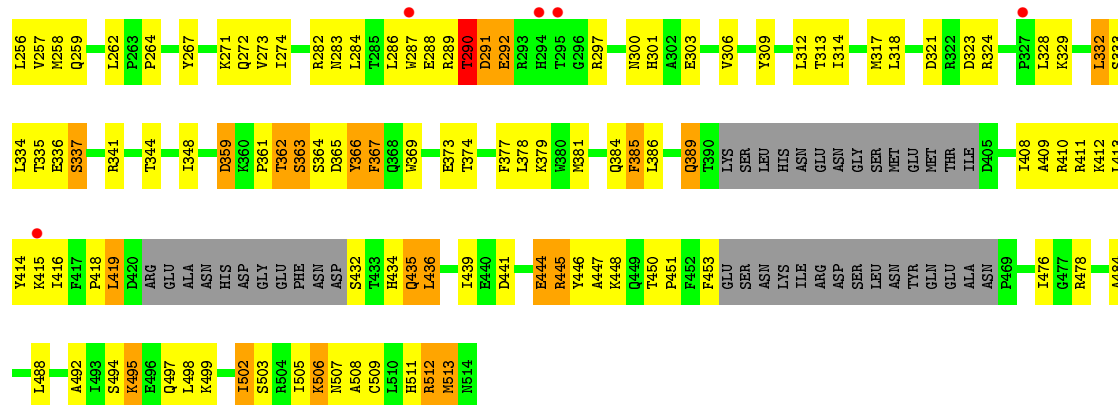


• Molecule 2: RNA polymerase I-specific transcription initiation factor RRN7

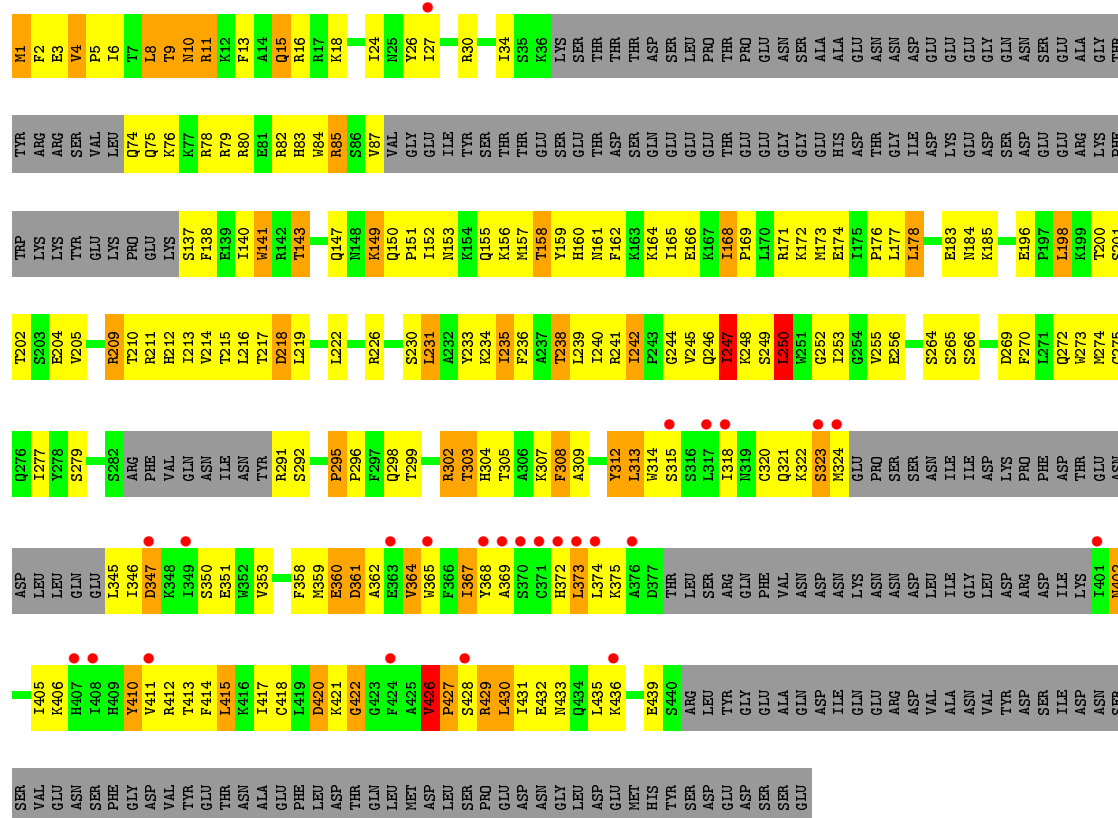
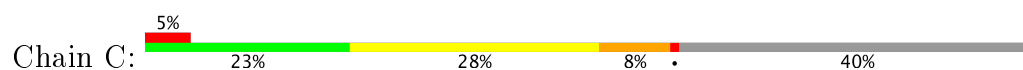


• Molecule 2: RNA polymerase I-specific transcription initiation factor RRN7

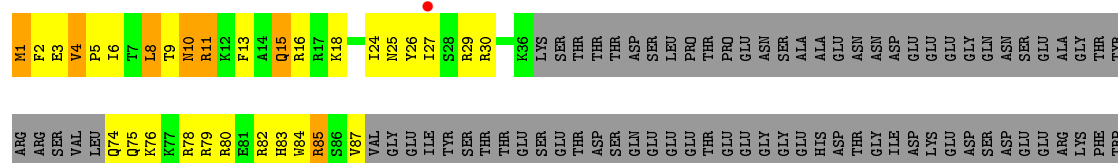
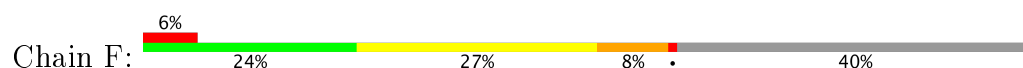


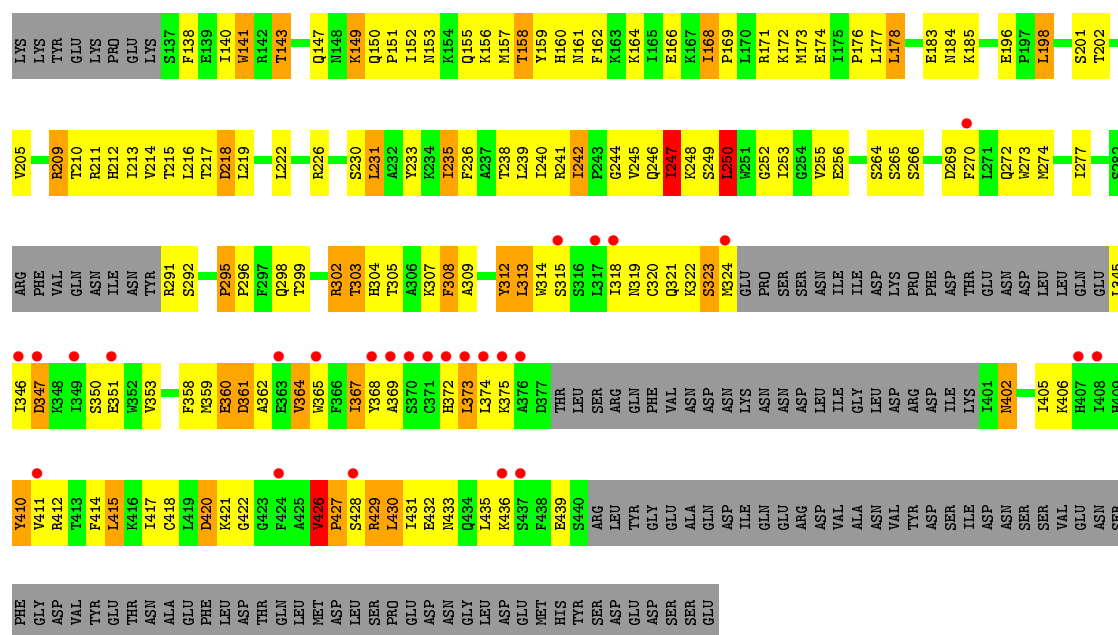


● Molecule 3: RNA polymerase I-specific transcription initiation factor RRN11

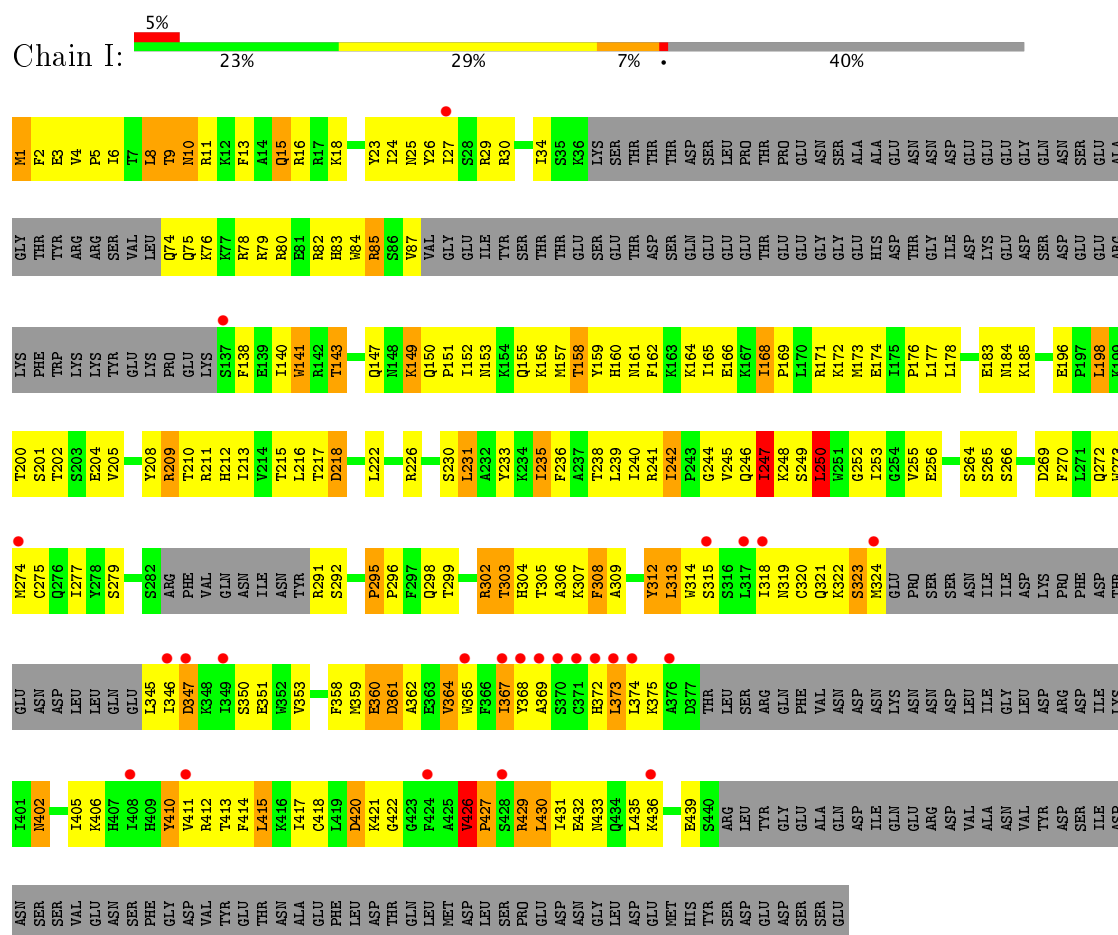


● Molecule 3: RNA polymerase I-specific transcription initiation factor RRN11

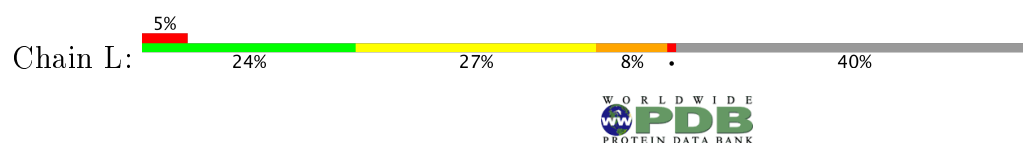


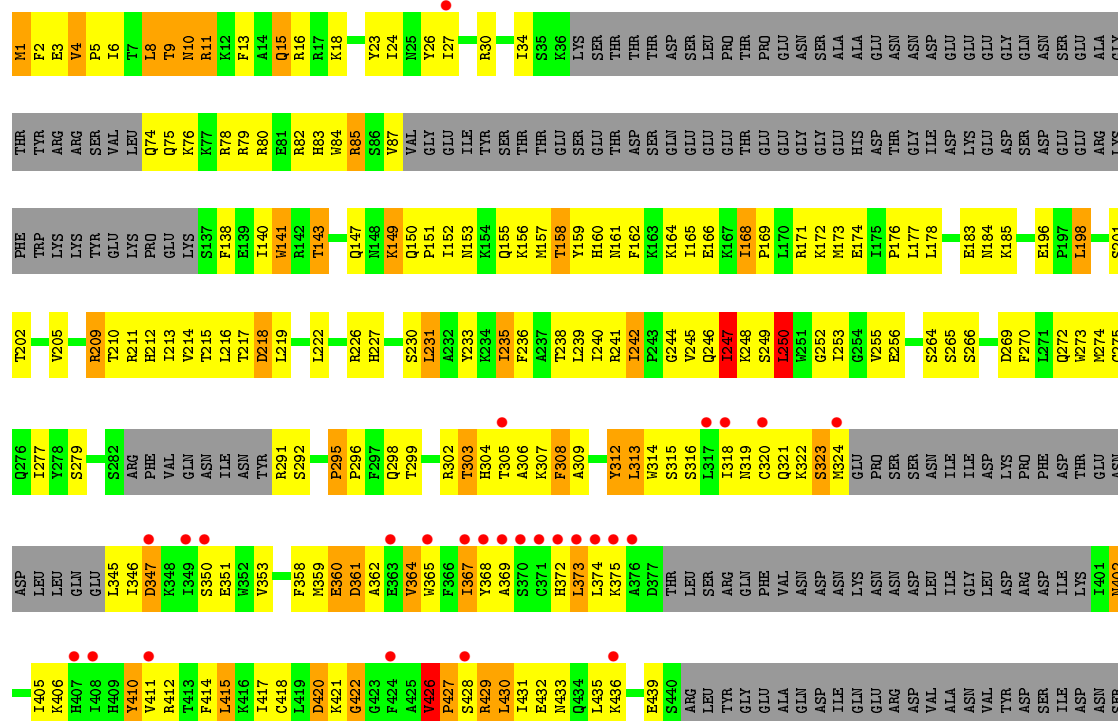
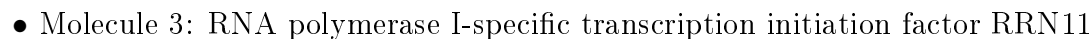


- Molecule 3: RNA polymerase I-specific transcription initiation factor RRN11



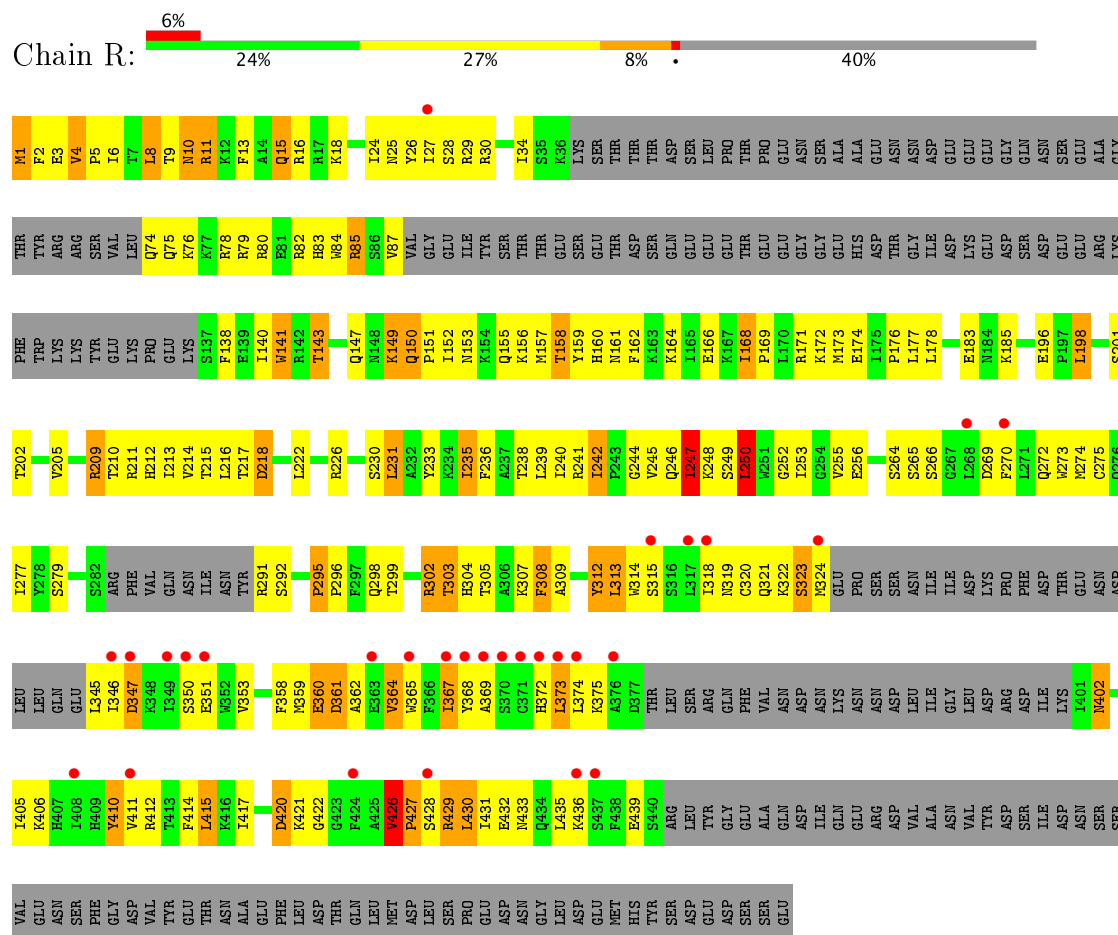
- Molecule 3: RNA polymerase I-specific transcription initiation factor RRN11





SER	VAL	GLU	ASN	SER	PHE	GLY	ASP	VAL	TYR	GLU	THR	ASN	ALA	GLU	PHE	LEU	ASP	THR	GLN	LEU	MET	ASP	LEU	SER	PRO	GLU	ASP	ASN	GLY	LEU	ASP	GLU	MET	HIS	TYR	SER	ASP	GLU	ASP	SER	SER	GLU
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

- 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) 98.9 (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 0.253 , 0.282	Depositor DCC
R_{free} test set	7456 reflections (2.97%)	DCC
Wilson B-factor (Å ²)	127.2	Xtriage
Anisotropy	0.203	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 129.6	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 [i](#)

5.1 Standard geometry [i](#)

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:M: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
2:Q:113:LYS:HG3	2:Q:134:LYS:HZ1	1.61	0.65
1:P:698:LYS:HE2	2:Q:124:ARG:HH21	1.62	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:49:THR:HB	3:C:318:ILE:HG21	1.79	0.64
1:A:717:LYS:NZ	4:A:1005:SO4:O1	2.28	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:346:ILE:HD12	3:F:375:LYS:HD3	1.83	0.60
3:F:359:MET:N	3:F:359:MET:SD	2.74	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:253:ILE:HA	3:O:256:GLU:HB3	1.84	0.60
3:O:250:LEU:HB2	3:O:270:PHE:HE2	1.66	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:253:ILE:HA	3:C:256:GLU:HB3	1.85	0.59
3:C:250:LEU:HB2	3:C:270:PHE:HE2	1.66	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:420:GLU:HA	1:J:442:LEU:O	2.04	0.58
1:J:174:TRP:HB3	3:L:198:LEU:HD23	1.85	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:174:TRP:HB3	3:I:198:LEU:HD23	1.85	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: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
2:B:274:ILE:HG23	2:B:282:ARG:HH22	1.69	0.57
1:A:725:VAL:HG21	2:B:446:TYR:CD1	2.39	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:251:SER:HB3	1:P:411:LYS:HD2	1.86	0.57
1:P:317:ILE:HG22	1:P:363:ILE:HD13	1.84	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:656:HIS:HB2	1:J:747:LEU:O	2.05	0.56
1:J:665:ASN:OD1	1:J:665:ASN:N	2.34	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
1:J:725:VAL:HG21	2:K:446:TYR:CD1	2.40	0.56
2:K:286:LEU:HD22	2:K:300:ASN:HB3	1.87	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:318:LEU:HB3	2:B:476:ILE:HD12	1.89	0.55
2:B:337:SER:HB2	2:B:448:LYS:HD3	1.87	0.55
1:D:384:ASP:OD2	1:D:387:ASN:HB2	2.07	0.55
1:D:251:SER:HB3	1:D:411:LYS:HD2	1.87	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:198:ILE:HG21	2:K:389:GLN:HA	1.89	0.54
2:K:257:VAL:HG13	2:K:262:LEU:HB2	1.88	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
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
1:M:599:LYS:HE3	2:N:272:GLN:HE22	1.71	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:715:TYR:CE1	1:M:733:THR:HG23	2.42	0.54
1:M:675:PHE:CZ	1:M:742:TRP:HZ3	2.25	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:389:TRP:CH2	3:F:147:GLN:HA	2.43	0.53
1:D:659:LEU:HD12	1:D:742:TRP:CD1	2.42	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:318:LEU:HB3	2:E:476:ILE:HD12	1.89	0.53
2:E:333:SER:HA	2:E:336:GLU:HG2	1.90	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:631:SER:O	1:D:686:TYR:OH	2.26	0.53
1:D:675:PHE:CZ	1:D:742:TRP:HZ3	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
1:G:389:TRP:CH2	3:I:147:GLN:HA	2.43	0.52
2:H:101:LYS:O	2:H:105:LEU:HG	2.09	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:599:LYS:HE3	2:E:272:GLN:HE22	1.73	0.52
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
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:198:ILE:HG21	2:H:389:GLN:HA	1.92	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
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:301:GLN:N	1:D:319:ASP:O	2.42	0.51
1:D:292:LEU:CD1	1:D:343:LEU:HG	2.40	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:26:TYR:CB	3:R:169:PRO:HB3	2.41	0.50
3:R:209:ARG:H	3:R:209:ARG:HD3	1.76	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:26:TYR:CB	3:O:169:PRO:HB3	2.41	0.50
3:O:177:LEU:HD22	3:O:185:LYS:HG2	1.93	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
2:N:137:TRP:CE3	2:N:140:ILE:HD11	2.48	0.48
1:M:656:HIS:CE1	2:N:171:HIS:CE1	3.00	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
1:P:573:GLU:HB3	2:Q:499:LYS:HD3	1.96	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
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:751:SER:O	1:J:753:PHE:N	2.46	0.47
1:J:656:HIS:CE1	2:K:171:HIS:CE1	3.03	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:171:ARG:HH22	2:N:444:GLU:HG2	1.79	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
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
1:M:573:GLU:HB3	2:N:499:LYS:HD3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:367:PHE:CE2	3:O:222:LEU:HD21	2.49	0.47
2:N:414:TYR:HE2	2:N:419:LEU:HB3	1.80	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: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
1:A:656:HIS:CE1	2:B:171:HIS:CE1	3.02	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: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
1:P:650:LEU:HD22	2:Q:242:PHE:HA	1.98	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
1:P:355:GLU:HA	3:R:24:ILE:HD12	1.97	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: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:137:TRP:O	2:H:141:LEU:HB2	2.16	0.46
2:H:105:LEU:HD13	2:H:141:LEU:HD11	1.97	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:96:ILE:HB	2:N:100:ALA:HB2	1.98	0.46
2:N:239:PHE:HB2	2:N:245:SER:OG	2.16	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
2:E:108:PHE:CD1	2:E:156:LEU:HB3	2.51	0.45
1:D:573:GLU:HB3	2:E:499:LYS:HD3	1.98	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:656:HIS:N	1:J:656:HIS:CD2	2.84	0.45
1:J:650:LEU:HD22	2:K:242:PHE:HA	1.98	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:9:THR:O	3:O:13:PHE:HD2	2.00	0.45
3:O:158:THR:HG23	3:O:161:ASN:H	1.80	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:619:GLU:OE2	1:A:670:ALA:N	2.49	0.45
1:A:660:LYS:HA	1:A:660:LYS:HD3	1.66	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
2:E:386:LEU:HD13	3:F:241:ARG:NH2	2.32	0.45
3:F:231:LEU:O	3:F:235:ILE:HG12	2.17	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
1:A:573:GLU:HB3	2:B:499:LYS:HD3	1.98	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
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:270:GLN:HG2	1:P:291:PRO:HB3	1.99	0.44
1:P:290:GLU:HG3	1:P:291:PRO:O	2.17	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:152:LEU:HD12	2:Q:154:LEU:HD11	1.99	0.44
2:Q:108:PHE:CD1	2:Q:156:LEU:HB3	2.51	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:239:PHE:CG	2:E:240:LYS:N	2.85	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:178:THR:HG22	2:E:303:GLU:OE1	2.17	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:221:PRO:HD2	2:B:222:PHE:CD2	2.52	0.44
2:B:178:THR:HG21	2:B:227:TYR:OH	2.18	0.44
3:F:27:ILE:HD11	3:F:166:GLU:HA	2.00	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
1:G:574:TRP:CH2	2:H:495:LYS:HD2	2.52	0.44
2:H:447:ALA:HA	2:H:450:THR:HB	1.98	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:96:ILE:HB	2:E:100:ALA:HB2	1.99	0.44
2:E:129:PHE:HE1	2:E:169:SER:N	2.16	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:394:VAL:HG21	3:O:143:THR:HG22	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:470:SER:O	1:M:504:THR:HG22	2.18	0.43
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
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
1:D:739:ASP:OD1	2:E:250:GLN:NE2	2.51	0.43
2:E:221:PRO:HD2	2:E:222:PHE:CD2	2.53	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: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
1:P:443:ASP:O	3:R:3:GLU:N	2.52	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:4:VAL:HG21	3:R:214:VAL:HG22	2.01	0.42
3:R:291:ARG:HG2	3:R:292:SER:H	1.84	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
1:J:394:VAL:HG21	3:L:143:THR:HG22	2.00	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: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:140:ILE:HG22	2:N:236:MET:HG2	2.01	0.42
2:N:221:PRO:HD2	2:N:222:PHE:HD2	1.84	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:129:PHE:HE1	2:B:169:SER:N	2.17	0.42
2:B:152:LEU:HB3	2:B:154:LEU:CD2	2.48	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
1:J:574:TRP:CH2	2:K:495:LYS:HD2	2.54	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
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:413:GLY:HA2	1:M:426:ALA:HB2	2.02	0.42
1:M:412:ASN:O	1:M:426:ALA:HB1	2.20	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
2:B:153:LYS:HB3	2:B:153:LYS:HE2	1.77	0.42
1:A:721:CYS:HB3	2:B:446:TYR:CD2	2.54	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:412:ASN:O	1:D:426:ALA:HB1	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:433:VAL:HG22	1:D:434:ARG:O	2.20	0.41
1:D:394:VAL:HG22	1:D:434:ARG:NH1	2.35	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:366:TYR:HA	2:H:369:TRP:CD1	2.54	0.41
2:H:341:ARG:HD3	2:H:373:GLU:OE2	2.20	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:290:GLU:HG2	1:G:342:GLN:HB2	2.01	0.41
1:G:329:ILE:HG13	1:G:330:PRO:N	2.33	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:390:GLN:HB2	3:C:151:PRO:O	2.20	0.41
1:A:408:ILE:HG23	1:A:413:GLY:C	2.40	0.41
2:B:386:LEU:HD13	3:C:241:ARG:NH2	2.34	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
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:34:ILE:HD12	3:O:34:ILE:HA	1.89	0.41
3:O:314:TRP:CD1	3:O:367:ILE:HD11	2.55	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:194:GLN:HG3	3:L:209:ARG:HH11	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:226:LEU:O	2:K:230:ILE:HG23	2.19	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:248:PRO:HB3	1:A:305:PHE:HB2	2.03	0.41
1:A:290:GLU:OE2	1:A:291:PRO:HD2	2.21	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:194:GLN:HG3	3:C:209:ARG:NH1	2.34	0.41
2:B:303:GLU:O	2:B:306:VAL:N	2.53	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: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
1:M:352:PHE:CE1	3:O:157:MET:HG2	2.56	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
1:P:721:CYS:HB3	2:Q:446:TYR:CD2	2.56	0.40
2:Q:262:LEU:HA	2:Q:262:LEU:HD23	1.87	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
1:G:443:ASP:O	3:I:3:GLU:N	2.55	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: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
1:M:55:LEU:HD23	3:O:227:HIS:CG	2.57	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
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	28
1	D	584/894 (65%)	500 (86%)	63 (11%)	21 (4%)	4	27
1	G	584/894 (65%)	500 (86%)	62 (11%)	22 (4%)	4	25
1	J	584/894 (65%)	500 (86%)	62 (11%)	22 (4%)	4	25
1	M	584/894 (65%)	498 (85%)	65 (11%)	21 (4%)	4	27
1	P	584/894 (65%)	499 (85%)	65 (11%)	20 (3%)	4	28
2	B	367/514 (71%)	323 (88%)	40 (11%)	4 (1%)	17	58
2	E	367/514 (71%)	321 (88%)	42 (11%)	4 (1%)	17	58
2	H	367/514 (71%)	320 (87%)	43 (12%)	4 (1%)	17	58
2	K	367/514 (71%)	322 (88%)	41 (11%)	4 (1%)	17	58
2	N	367/514 (71%)	322 (88%)	41 (11%)	4 (1%)	17	58
2	Q	367/514 (71%)	321 (88%)	42 (11%)	4 (1%)	17	58
3	C	291/507 (57%)	244 (84%)	40 (14%)	7 (2%)	7	39
3	F	291/507 (57%)	248 (85%)	37 (13%)	6 (2%)	8	42
3	I	291/507 (57%)	246 (84%)	39 (13%)	6 (2%)	8	42
3	L	291/507 (57%)	246 (84%)	39 (13%)	6 (2%)	8	42
3	O	291/507 (57%)	245 (84%)	39 (13%)	7 (2%)	7	39
3	R	291/507 (57%)	248 (85%)	37 (13%)	6 (2%)	8	42
All	All	7452/11490 (65%)	6402 (86%)	862 (12%)	188 (2%)	6	38

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	4
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	14
2	E	354/476 (74%)	297 (84%)	57 (16%)	3	13
2	H	354/476 (74%)	297 (84%)	57 (16%)	3	13
2	K	354/476 (74%)	297 (84%)	57 (16%)	3	13
2	N	354/476 (74%)	297 (84%)	57 (16%)	3	13
2	Q	354/476 (74%)	297 (84%)	57 (16%)	3	13
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	5
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

Continued on next page...

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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	0.26	0	6,6,6	0.22	0
4	SO4	A	1002	-	4,4,4	0.16	0	6,6,6	0.23	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	0.16	0	6,6,6	0.17	0
4	SO4	A	1004	-	4,4,4	0.16	0	6,6,6	0.09	0
4	SO4	A	1005	-	4,4,4	0.14	0	6,6,6	0.10	0
4	SO4	D	1001	-	4,4,4	0.26	0	6,6,6	0.21	0
4	SO4	D	1002	-	4,4,4	0.18	0	6,6,6	0.22	0
4	SO4	D	1003	-	4,4,4	0.15	0	6,6,6	0.11	0
4	SO4	D	1004	-	4,4,4	0.13	0	6,6,6	0.10	0
4	SO4	F	601	-	4,4,4	0.15	0	6,6,6	0.09	0
4	SO4	G	901	-	4,4,4	0.16	0	6,6,6	0.22	0
4	SO4	G	902	-	4,4,4	0.16	0	6,6,6	0.15	0
4	SO4	G	903	-	4,4,4	0.13	0	6,6,6	0.10	0
4	SO4	H	1001	-	4,4,4	0.27	0	6,6,6	0.25	0
4	SO4	I	601	-	4,4,4	0.16	0	6,6,6	0.10	0
4	SO4	J	1001	-	4,4,4	0.24	0	6,6,6	0.24	0
4	SO4	J	1002	-	4,4,4	0.16	0	6,6,6	0.16	0
4	SO4	J	1003	-	4,4,4	0.13	0	6,6,6	0.11	0
4	SO4	K	601	-	4,4,4	0.17	0	6,6,6	0.19	0
4	SO4	L	601	-	4,4,4	0.15	0	6,6,6	0.10	0
4	SO4	M	1001	-	4,4,4	0.23	0	6,6,6	0.34	0
4	SO4	M	1002	-	4,4,4	0.16	0	6,6,6	0.19	0
4	SO4	M	1003	-	4,4,4	0.16	0	6,6,6	0.14	0
4	SO4	M	1004	-	4,4,4	0.14	0	6,6,6	0.10	0
4	SO4	O	601	-	4,4,4	0.15	0	6,6,6	0.12	0
4	SO4	P	1001	-	4,4,4	0.25	0	6,6,6	0.32	0
4	SO4	P	1002	-	4,4,4	0.16	0	6,6,6	0.19	0
4	SO4	P	1003	-	4,4,4	0.17	0	6,6,6	0.13	0
4	SO4	P	1004	-	4,4,4	0.15	0	6,6,6	0.13	0
4	SO4	P	1005	-	4,4,4	0.14	0	6,6,6	0.10	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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(Å²)	Q<0.9
1	A	598/894 (66%)	0.31	33 (5%)	26	15	85, 143, 228, 326	0
1	D	598/894 (66%)	0.30	31 (5%)	28	16	86, 145, 228, 326	0
1	G	598/894 (66%)	0.31	29 (4%)	31	19	83, 145, 229, 339	0
1	J	598/894 (66%)	0.30	28 (4%)	32	19	85, 144, 226, 317	0
1	M	598/894 (66%)	0.30	31 (5%)	28	16	86, 146, 230, 331	0
1	P	598/894 (66%)	0.31	26 (4%)	36	23	86, 144, 230, 328	0
2	B	377/514 (73%)	0.20	12 (3%)	48	32	78, 128, 210, 294	0
2	E	377/514 (73%)	0.19	13 (3%)	46	30	79, 129, 217, 279	0
2	H	377/514 (73%)	0.18	12 (3%)	48	32	79, 128, 210, 283	0
2	K	377/514 (73%)	0.18	11 (2%)	52	37	79, 130, 214, 287	0
2	N	377/514 (73%)	0.17	11 (2%)	52	37	79, 127, 207, 284	0
2	Q	377/514 (73%)	0.19	12 (3%)	48	32	79, 129, 211, 286	0
3	C	303/507 (59%)	0.45	25 (8%)	12	7	82, 158, 242, 312	0
3	F	303/507 (59%)	0.48	28 (9%)	10	6	84, 158, 248, 318	0
3	I	303/507 (59%)	0.48	25 (8%)	12	7	83, 154, 241, 324	0
3	L	303/507 (59%)	0.45	25 (8%)	12	7	83, 160, 241, 326	0
3	O	303/507 (59%)	0.48	27 (8%)	10	6	84, 156, 244, 313	0
3	R	303/507 (59%)	0.46	29 (9%)	9	5	83, 155, 242, 334	0
All	All	7668/11490 (66%)	0.31	408 (5%)	27	15	78, 141, 230, 339	0

All (408) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	I	369	ALA	9.1
1	P	651	SER	7.6
3	I	428	SER	7.1

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Mol	Chain	Res	Type	RSRZ
3	C	369	ALA	7.0
1	M	651	SER	7.0
3	L	347	ASP	6.9
3	L	369	ALA	6.7
3	F	370	SER	6.6
1	D	501	PRO	6.6
3	O	369	ALA	6.5
3	O	408	ILE	6.5
3	F	347	ASP	6.4
3	L	408	ILE	6.3
1	A	651	SER	6.3
1	G	651	SER	6.2
3	I	370	SER	6.2
1	J	501	PRO	6.2
3	R	369	ALA	6.1
3	O	347	ASP	6.1
1	J	651	SER	6.0
3	C	370	SER	6.0
3	R	408	ILE	6.0
2	B	294	HIS	5.6
3	F	408	ILE	5.6
3	C	408	ILE	5.5
1	A	501	PRO	5.5
3	R	347	ASP	5.4
1	M	462	ILE	5.4
3	R	370	SER	5.4
1	G	501	PRO	5.3
3	F	369	ALA	5.3
1	P	501	PRO	5.3
3	L	370	SER	5.3
1	J	196	TYR	5.3
1	D	196	TYR	5.2
3	I	347	ASP	5.2
1	M	501	PRO	5.2
1	D	651	SER	5.1
1	A	462	ILE	5.1
1	P	502	GLY	5.1
2	E	294	HIS	5.0
3	O	370	SER	5.0
3	C	347	ASP	5.0
1	A	502	GLY	4.9
1	G	532	GLU	4.9

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Mol	Chain	Res	Type	RSRZ
3	I	324	MET	4.9
1	D	532	GLU	4.7
3	I	411	VAL	4.7
3	L	411	VAL	4.7
1	D	502	GLY	4.7
1	J	532	GLU	4.6
3	C	324	MET	4.5
3	O	376	ALA	4.5
1	G	462	ILE	4.5
3	F	428	SER	4.5
1	G	502	GLY	4.5
1	J	502	GLY	4.5
1	M	532	GLU	4.4
1	A	532	GLU	4.4
3	I	408	ILE	4.4
1	G	237	GLU	4.4
3	C	428	SER	4.3
2	Q	156	LEU	4.3
3	C	411	VAL	4.3
1	D	462	ILE	4.3
3	F	411	VAL	4.2
3	O	428	SER	4.2
1	J	654	LEU	4.2
2	H	294	HIS	4.1
1	P	196	TYR	4.1
3	R	411	VAL	4.1
3	O	324	MET	4.1
3	R	372	HIS	4.1
3	R	373	LEU	4.1
2	Q	287	TRP	4.0
2	K	156	LEU	4.0
3	I	376	ALA	4.0
1	J	503	GLY	4.0
1	M	289	SER	3.9
3	C	365	TRP	3.9
1	G	289	SER	3.9
3	L	428	SER	3.9
1	G	196	TYR	3.9
2	N	294	HIS	3.9
2	H	198	ILE	3.9
1	J	462	ILE	3.9
1	P	462	ILE	3.8

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Mol	Chain	Res	Type	RSRZ
3	O	411	VAL	3.8
2	B	287	TRP	3.8
3	R	374	LEU	3.8
1	M	502	GLY	3.8
3	O	372	HIS	3.8
2	H	156	LEU	3.8
3	F	324	MET	3.8
1	M	237	GLU	3.8
3	L	376	ALA	3.8
3	I	368	TYR	3.8
2	K	294	HIS	3.8
2	N	156	LEU	3.7
3	L	368	TYR	3.7
2	E	287	TRP	3.7
2	K	198	ILE	3.7
1	A	237	GLU	3.7
3	F	376	ALA	3.7
1	A	289	SER	3.7
3	R	365	TRP	3.6
2	Q	294	HIS	3.6
3	F	365	TRP	3.6
3	C	376	ALA	3.6
2	K	327	PRO	3.6
1	D	237	GLU	3.6
3	R	324	MET	3.6
2	N	327	PRO	3.6
3	L	365	TRP	3.6
3	F	424	PHE	3.5
3	C	372	HIS	3.5
3	L	372	HIS	3.5
1	J	445	ASP	3.5
3	L	318	ILE	3.5
3	O	365	TRP	3.5
1	A	304	ASP	3.5
1	P	532	GLU	3.5
3	R	428	SER	3.4
1	P	237	GLU	3.4
2	B	198	ILE	3.4
2	H	152	LEU	3.4
3	F	368	TYR	3.4
3	C	374	LEU	3.4
3	F	315	SER	3.4

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Mol	Chain	Res	Type	RSRZ
3	L	349	ILE	3.4
1	P	503	GLY	3.4
3	I	371	CYS	3.4
3	C	315	SER	3.3
2	K	287	TRP	3.3
3	I	374	LEU	3.3
3	I	372	HIS	3.3
3	I	436	LYS	3.3
3	I	365	TRP	3.3
3	R	376	ALA	3.3
3	L	374	LEU	3.3
3	O	374	LEU	3.3
3	R	317	LEU	3.3
1	G	272	PHE	3.3
1	J	237	GLU	3.3
3	O	368	TYR	3.3
3	F	374	LEU	3.3
3	F	372	HIS	3.3
3	R	436	LYS	3.3
1	G	654	LEU	3.2
3	C	368	TYR	3.2
3	L	324	MET	3.2
1	P	261	VAL	3.2
2	N	287	TRP	3.2
3	R	368	TYR	3.1
3	R	346	ILE	3.1
1	A	196	TYR	3.1
3	I	318	ILE	3.1
3	R	27	ILE	3.1
2	E	327	PRO	3.1
1	A	225	LEU	3.1
3	O	371	CYS	3.1
3	C	373	LEU	3.1
3	L	373	LEU	3.1
2	Q	327	PRO	3.0
1	A	272	PHE	3.0
1	M	224	THR	3.0
1	P	456	VAL	3.0
3	C	371	CYS	3.0
2	N	198	ILE	3.0
1	D	281	SER	3.0
3	L	436	LYS	3.0

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Mol	Chain	Res	Type	RSRZ
1	D	289	SER	3.0
1	J	289	SER	3.0
2	E	198	ILE	3.0
3	F	371	CYS	3.0
3	L	424	PHE	3.0
2	H	287	TRP	3.0
1	G	445	ASP	3.0
3	I	27	ILE	3.0
3	I	424	PHE	3.0
1	D	236	ILE	3.0
1	D	654	LEU	3.0
2	Q	152	LEU	3.0
3	F	318	ILE	2.9
1	M	272	PHE	2.9
1	M	445	ASP	2.9
3	I	317	LEU	2.9
1	D	503	GLY	2.9
3	L	371	CYS	2.9
2	Q	198	ILE	2.9
1	A	445	ASP	2.9
1	P	445	ASP	2.9
2	H	327	PRO	2.9
3	O	317	LEU	2.8
3	R	349	ILE	2.8
2	E	129	PHE	2.8
3	C	436	LYS	2.8
1	D	272	PHE	2.8
1	A	503	GLY	2.8
3	C	318	ILE	2.8
3	O	363	GLU	2.8
1	P	304	ASP	2.8
1	J	456	VAL	2.8
1	P	654	LEU	2.8
2	N	152	LEU	2.8
3	I	373	LEU	2.8
1	D	456	VAL	2.8
1	P	272	PHE	2.8
1	A	236	ILE	2.8
1	A	263	ILE	2.8
1	M	196	TYR	2.8
3	C	323	SER	2.7
3	R	318	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
3	C	317	LEU	2.7
3	L	317	LEU	2.7
3	L	346	ILE	2.7
2	N	129	PHE	2.7
3	F	349	ILE	2.7
3	F	317	LEU	2.7
1	D	457	LYS	2.7
3	O	27	ILE	2.7
2	B	327	PRO	2.7
3	F	436	LYS	2.7
1	M	456	VAL	2.7
3	R	424	PHE	2.7
3	O	407	HIS	2.7
1	M	236	ILE	2.7
2	B	156	LEU	2.6
1	D	444	PRO	2.6
1	P	289	SER	2.6
1	J	261	VAL	2.6
2	B	135	ILE	2.6
1	J	272	PHE	2.6
1	J	304	ASP	2.6
1	D	304	ASP	2.6
2	E	156	LEU	2.6
1	A	444	PRO	2.6
1	J	457	LYS	2.6
3	I	367	ILE	2.6
3	R	371	CYS	2.6
3	F	346	ILE	2.6
3	I	349	ILE	2.6
2	K	152	LEU	2.6
3	O	436	LYS	2.6
3	F	373	LEU	2.6
3	O	349	ILE	2.6
3	O	424	PHE	2.5
1	G	549	TYR	2.5
3	R	367	ILE	2.5
1	G	483	HIS	2.5
1	P	227	LEU	2.5
3	O	373	LEU	2.5
1	J	549	TYR	2.5
1	M	483	HIS	2.5
2	H	115	GLN	2.5

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Mol	Chain	Res	Type	RSRZ
1	G	236	ILE	2.5
2	N	136	ILE	2.5
3	C	424	PHE	2.5
3	C	401	ILE	2.5
3	F	270	PHE	2.5
3	I	346	ILE	2.5
1	A	483	HIS	2.5
2	Q	129	PHE	2.5
1	G	224	THR	2.5
1	A	654	LEU	2.4
1	P	214	LEU	2.4
2	B	129	PHE	2.4
1	D	445	ASP	2.4
1	M	218	VAL	2.4
1	D	261	VAL	2.4
1	J	236	ILE	2.4
2	E	136	ILE	2.4
2	K	138	LEU	2.4
3	R	270	PHE	2.4
3	O	375	LYS	2.4
1	J	227	LEU	2.4
2	B	139	LYS	2.4
1	D	227	LEU	2.4
3	O	320	CYS	2.4
1	M	428	GLU	2.4
1	P	428	GLU	2.4
3	O	367	ILE	2.4
1	D	264	ILE	2.4
1	A	456	VAL	2.4
1	M	654	LEU	2.4
3	R	315	SER	2.4
1	P	236	ILE	2.4
2	K	142	LYS	2.4
1	A	224	THR	2.4
3	F	407	HIS	2.4
1	M	281	SER	2.4
2	B	94	LYS	2.4
2	N	142	LYS	2.4
1	A	205	TYR	2.3
1	A	227	LEU	2.3
1	M	219	LEU	2.3
3	I	315	SER	2.3

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Mol	Chain	Res	Type	RSRZ
1	G	503	GLY	2.3
3	F	363	GLU	2.3
2	E	152	LEU	2.3
2	Q	238	HIS	2.3
3	C	407	HIS	2.3
1	G	494	CYS	2.3
1	D	276	SER	2.3
2	B	152	LEU	2.3
2	E	295	THR	2.3
3	O	318	ILE	2.3
1	A	247	ILE	2.3
1	M	227	LEU	2.3
1	M	543	ASN	2.3
2	Q	295	THR	2.3
1	G	281	SER	2.3
1	G	698	LYS	2.2
1	J	263	ILE	2.2
3	F	437	SER	2.2
1	M	698	LYS	2.2
1	A	281	SER	2.2
1	J	281	SER	2.2
1	D	533	LEU	2.2
3	R	437	SER	2.2
1	A	770	ASP	2.2
1	J	233	VAL	2.2
2	Q	115	GLN	2.2
2	K	330	TRP	2.2
3	O	350	SER	2.2
1	A	264	ILE	2.2
1	M	247	ILE	2.2
3	I	274	MET	2.2
3	L	315	SER	2.2
1	A	549	TYR	2.2
1	A	233	VAL	2.2
1	M	759	GLU	2.2
1	M	225	LEU	2.2
1	M	444	PRO	2.2
1	D	263	ILE	2.2
2	H	135	ILE	2.2
1	D	652	GLY	2.2
1	A	533	LEU	2.2
2	K	238	HIS	2.2

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Mol	Chain	Res	Type	RSRZ
3	O	305	THR	2.2
1	A	550	TYR	2.2
1	D	699	LEU	2.2
1	G	225	LEU	2.2
3	F	375	LYS	2.2
2	H	138	LEU	2.1
3	R	268	LEU	2.1
1	G	263	ILE	2.1
3	C	349	ILE	2.1
1	D	233	VAL	2.1
1	J	224	THR	2.1
2	B	115	GLN	2.1
3	F	27	ILE	2.1
1	M	463	LEU	2.1
2	B	138	LEU	2.1
2	E	135	ILE	2.1
1	P	225	LEU	2.1
3	L	137	SER	2.1
3	L	437	SER	2.1
1	P	698	LYS	2.1
1	G	233	VAL	2.1
1	G	755	PRO	2.1
2	Q	211	TYR	2.1
1	D	483	HIS	2.1
1	D	247	ILE	2.1
1	G	227	LEU	2.1
1	M	503	GLY	2.1
2	E	138	LEU	2.1
1	D	271	ILE	2.1
1	J	247	ILE	2.1
1	P	187	ILE	2.1
2	E	330	TRP	2.1
1	M	457	LYS	2.1
2	H	94	LYS	2.1
1	M	214	LEU	2.1
1	J	216	ILE	2.1
1	P	216	ILE	2.1
1	P	494	CYS	2.1
2	K	135	ILE	2.1
3	C	27	ILE	2.1
3	R	350	SER	2.1
1	P	239	HIS	2.1

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Mol	Chain	Res	Type	RSRZ
1	J	264	ILE	2.1
1	A	214	LEU	2.1
3	I	137	SER	2.1
2	E	449	GLN	2.1
2	Q	415	LYS	2.1
3	C	363	GLU	2.1
3	L	81	GLU	2.1
3	R	363	GLU	2.1
1	G	214	LEU	2.1
2	H	318	LEU	2.1
1	P	444	PRO	2.0
1	D	461	HIS	2.0
1	G	759	GLU	2.0
1	A	216	ILE	2.0
1	A	698	LYS	2.0
1	M	304	ASP	2.0
2	N	330	TRP	2.0
1	G	444	PRO	2.0
3	L	305	THR	2.0
1	J	428	GLU	2.0
3	F	351	GLU	2.0
3	R	351	GLU	2.0
2	H	238	HIS	2.0
2	N	363	SER	2.0
1	G	247	ILE	2.0
1	G	274	ILE	2.0
1	J	444	PRO	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains.

The B-factors column lists the minimum, median, 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	LLDF	B-factors(Å ²)	Q<0.9
4	SO4	A	1001	5/5	0.96	0.43	6.36	96,110,115,123	0
4	SO4	O	601	5/5	0.94	0.52	6.25	101,215,246,246	0
4	SO4	F	601	5/5	0.95	0.52	6.10	99,179,235,237	0
4	SO4	A	1004	5/5	0.95	0.48	5.87	95,186,233,252	0
4	SO4	M	1001	5/5	0.96	0.46	5.58	92,110,119,130	0
4	SO4	P	1001	5/5	0.97	0.46	5.00	94,105,113,126	0
4	SO4	H	1001	5/5	0.98	0.42	4.91	92,92,108,112	0
4	SO4	I	601	5/5	0.94	0.49	4.69	98,191,239,244	0
4	SO4	J	1001	5/5	0.98	0.44	4.55	94,108,113,120	0
4	SO4	P	1004	5/5	0.95	0.44	4.26	96,187,207,226	0
4	SO4	D	1001	5/5	0.96	0.39	3.65	94,106,110,111	0
4	SO4	L	601	5/5	0.94	0.48	3.58	101,201,236,237	0
4	SO4	P	1002	5/5	0.80	0.33	3.42	166,168,172,186	0
4	SO4	M	1002	5/5	0.81	0.29	2.89	169,171,179,191	0
4	SO4	K	601	5/5	0.81	0.33	2.86	165,172,176,184	0
4	SO4	D	1002	5/5	0.89	0.32	2.82	144,165,173,183	0
4	SO4	G	901	5/5	0.88	0.32	2.62	153,155,162,180	0
4	SO4	A	1002	5/5	0.86	0.32	1.91	163,169,175,184	0
4	SO4	M	1004	5/5	0.66	0.29	1.74	164,293,328,365	0
4	SO4	A	1005	5/5	0.78	0.25	0.83	161,270,297,338	0
4	SO4	D	1004	5/5	0.77	0.25	0.72	172,284,325,366	0
4	SO4	J	1003	5/5	0.70	0.23	0.36	166,284,321,362	0
4	SO4	G	903	5/5	0.66	0.21	-0.26	164,281,309,354	0
4	SO4	M	1003	5/5	0.90	0.22	-0.49	107,162,234,240	0
4	SO4	P	1005	5/5	0.73	0.20	-0.49	166,296,344,363	0
4	SO4	P	1003	5/5	0.89	0.21	-0.63	111,150,158,158	0
4	SO4	J	1002	5/5	0.92	0.19	-0.66	106,127,143,149	0
4	SO4	G	902	5/5	0.90	0.21	-0.71	117,133,146,149	0
4	SO4	D	1003	5/5	0.90	0.20	-0.93	104,134,141,147	0
4	SO4	A	1003	5/5	0.87	0.20	-0.95	98,142,149,150	0
5	MG	J	1004	1/1	0.92	0.39	-	106,106,106,106	0
5	MG	G	904	1/1	0.94	0.34	-	108,108,108,108	0
5	MG	A	1006	1/1	0.84	0.38	-	107,107,107,107	0
5	MG	P	1006	1/1	0.86	0.35	-	108,108,108,108	0
5	MG	M	1005	1/1	0.93	0.37	-	108,108,108,108	0
5	MG	D	1005	1/1	0.91	0.31	-	107,107,107,107	0

6.5 Other polymers [i](#)

There are no such residues in this entry.