



Full wwPDB X-ray Structure Validation Report

May 15, 2020 – 09:44 am BST

PDB ID : 6QPF
Title : Influenza A virus Polymerase Heterotrimer A/duck/Fujian/01/2002(H5N1)
Authors : Fan, H.T.; Keown, J.R.; Fodor, E.; Grimes, J.M.
Deposited on : 2019-02-13
Resolution : 3.63 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the  symbol.

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

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.11
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

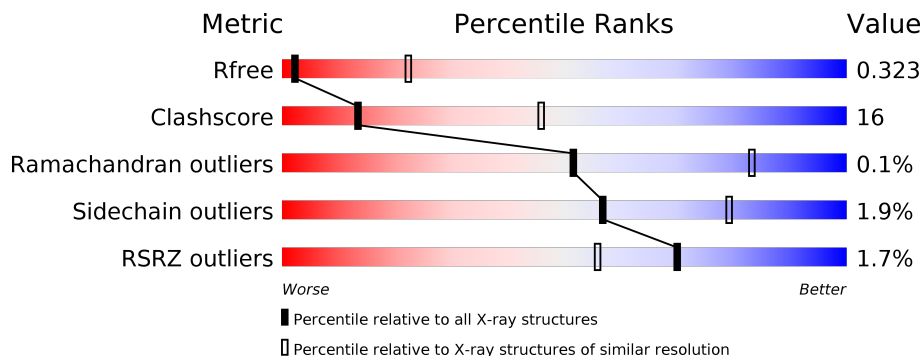
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.63 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}	130704	1341 (3.78-3.50)
Clashscore	141614	1439 (3.78-3.50)
Ramachandran outliers	138981	1391 (3.78-3.50)
Sidechain outliers	138945	1391 (3.78-3.50)
RSRZ outliers	127900	1242 (3.78-3.50)

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 respectively. 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	716	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 62%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 36%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: grey;"></div> </div> <p style="font-size: small; margin-top: 5px;">% 62% 36% .</p>
1	D	716	<div style="display: flex; align-items: center;"> <div style="width: 3%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 67%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 32%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: grey;"></div> </div> <p style="font-size: small; margin-top: 5px;">3% 67% 32% .</p>
1	G	716	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 64%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 35%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: grey;"></div> </div> <p style="font-size: small; margin-top: 5px;">% 64% 35% .</p>
1	J	716	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 63%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 34%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: grey;"></div> </div> <p style="font-size: small; margin-top: 5px;">2% 63% 34% ..</p>
2	B	757	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 57%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 33%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 10%; height: 10px; background-color: grey;"></div> </div> <p style="font-size: small; margin-top: 5px;">2% 57% 33% . 10%</p>
2	E	757	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 54%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 33%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 13%; height: 10px; background-color: grey;"></div> </div> <p style="font-size: small; margin-top: 5px;">2% 54% 33% . 13%</p>

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Mol	Chain	Length	Quality of chain
2	H	757	<p>% 56% 33% 11%</p>
2	K	757	<p>% 53% 34% 13%</p>
3	C	765	<p>2% 65% 29% 5%</p>
3	F	765	<p>3% 64% 31% 5%</p>
3	I	765	<p>2% 63% 31% 6%</p>
3	L	765	<p>% 60% 35% 5%</p>

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 67760 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 Polymerase acidic protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	716	Total	C	N	O	S	0	0	0
			5796	3671	985	1099	41			
1	D	716	Total	C	N	O	S	0	0	0
			5796	3671	985	1099	41			
1	G	716	Total	C	N	O	S	0	0	0
			5796	3671	985	1099	41			
1	J	710	Total	C	N	O	S	0	0	0
			5751	3643	978	1089	41			

- Molecule 2 is a protein called RNA-directed RNA polymerase catalytic subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	685	Total	C	N	O	S	0	0	0
			5474	3446	950	1037	41			
2	E	661	Total	C	N	O	S	0	0	0
			5283	3328	909	1005	41			
2	H	673	Total	C	N	O	S	0	0	0
			5389	3393	936	1020	40			
2	K	662	Total	C	N	O	S	0	0	0
			5290	3339	913	998	40			

- Molecule 3 is a protein called Polymerase basic protein 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	727	Total	C	N	O	S	0	0	0
			5790	3643	1042	1066	39			
3	F	731	Total	C	N	O	S	0	0	0
			5824	3661	1050	1074	39			
3	I	722	Total	C	N	O	S	0	0	0
			5755	3620	1038	1058	39			
3	L	730	Total	C	N	O	S	0	0	0
			5816	3657	1048	1072	39			

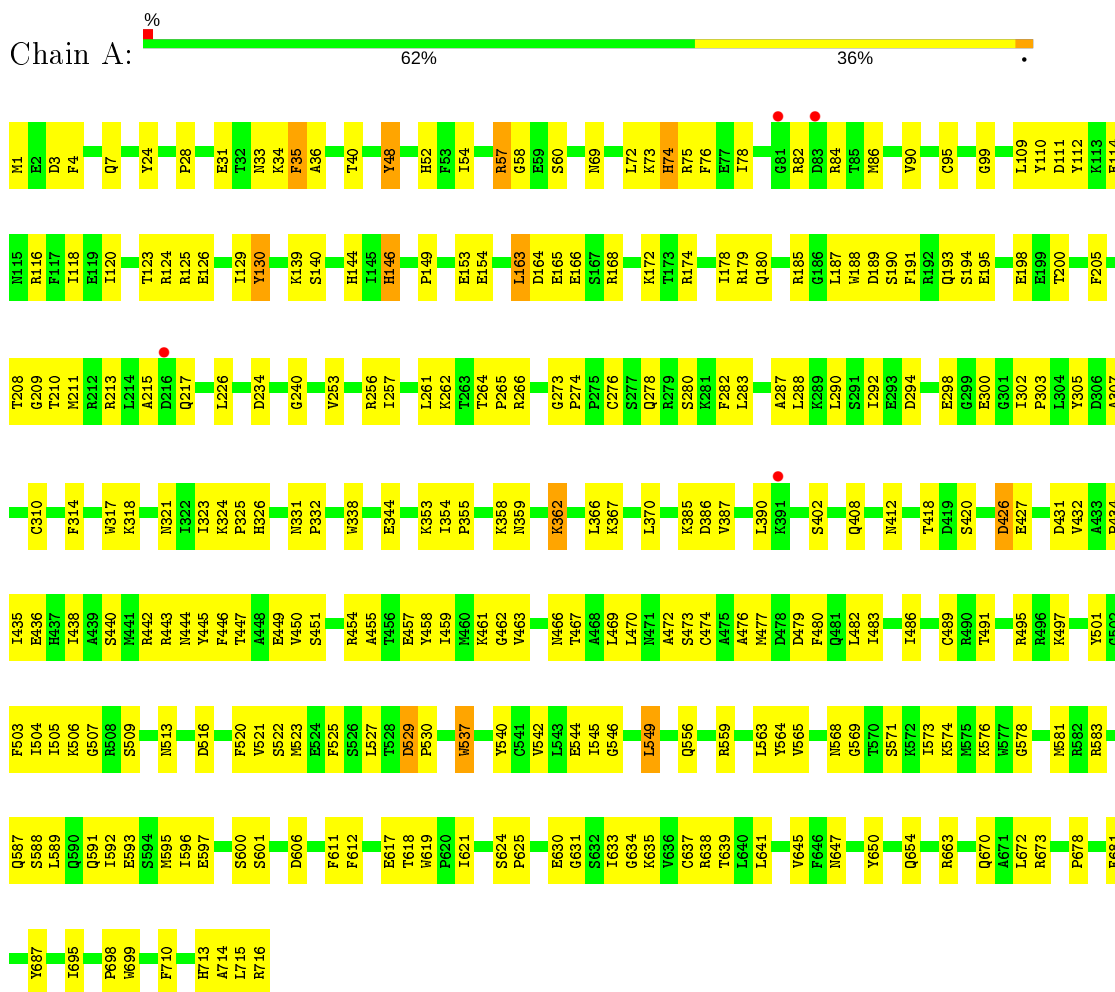
There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	760	GLU	-	expression tag	UNP D3YNB5
C	761	ASN	-	expression tag	UNP D3YNB5
C	762	LEU	-	expression tag	UNP D3YNB5
C	763	TYR	-	expression tag	UNP D3YNB5
C	764	PHE	-	expression tag	UNP D3YNB5
C	765	GLN	-	expression tag	UNP D3YNB5
F	760	GLU	-	expression tag	UNP D3YNB5
F	761	ASN	-	expression tag	UNP D3YNB5
F	762	LEU	-	expression tag	UNP D3YNB5
F	763	TYR	-	expression tag	UNP D3YNB5
F	764	PHE	-	expression tag	UNP D3YNB5
F	765	GLN	-	expression tag	UNP D3YNB5
I	760	GLU	-	expression tag	UNP D3YNB5
I	761	ASN	-	expression tag	UNP D3YNB5
I	762	LEU	-	expression tag	UNP D3YNB5
I	763	TYR	-	expression tag	UNP D3YNB5
I	764	PHE	-	expression tag	UNP D3YNB5
I	765	GLN	-	expression tag	UNP D3YNB5
L	760	GLU	-	expression tag	UNP D3YNB5
L	761	ASN	-	expression tag	UNP D3YNB5
L	762	LEU	-	expression tag	UNP D3YNB5
L	763	TYR	-	expression tag	UNP D3YNB5
L	764	PHE	-	expression tag	UNP D3YNB5
L	765	GLN	-	expression tag	UNP D3YNB5

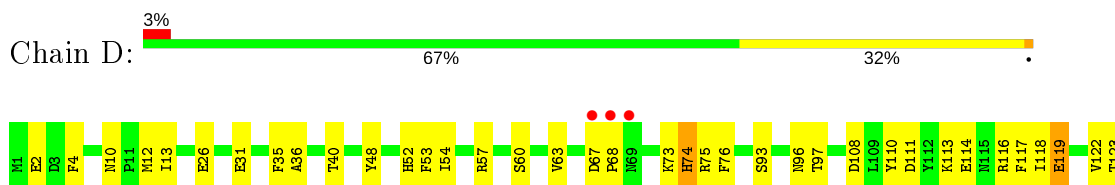
3 Residue-property plots

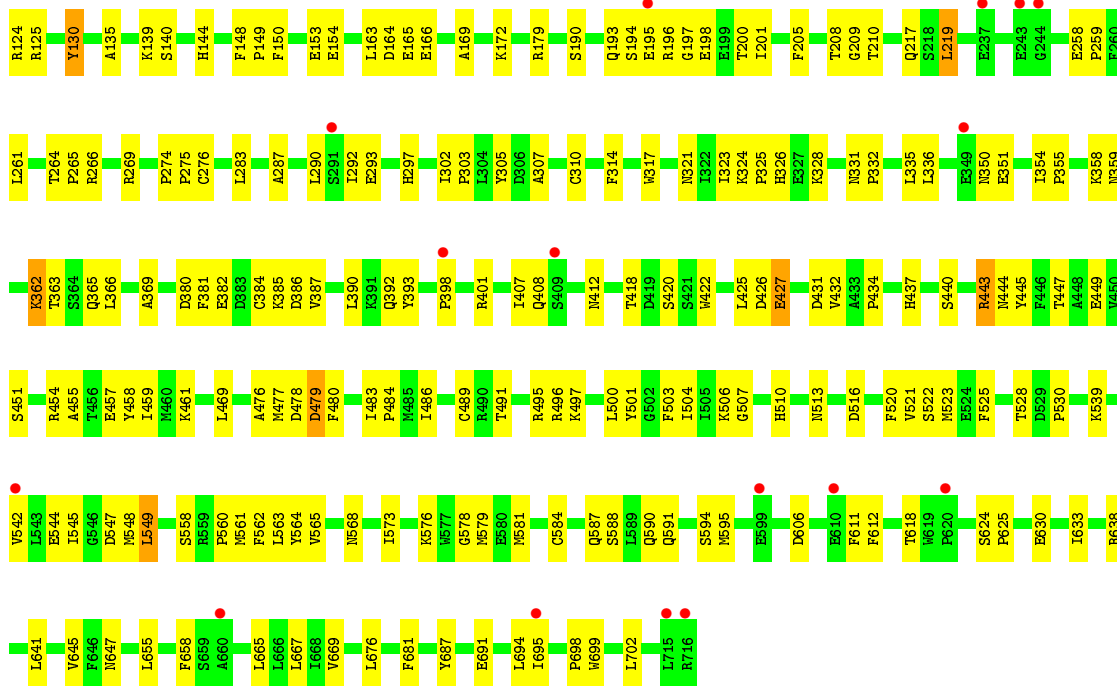
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

- Molecule 1: Polymerase acidic protein

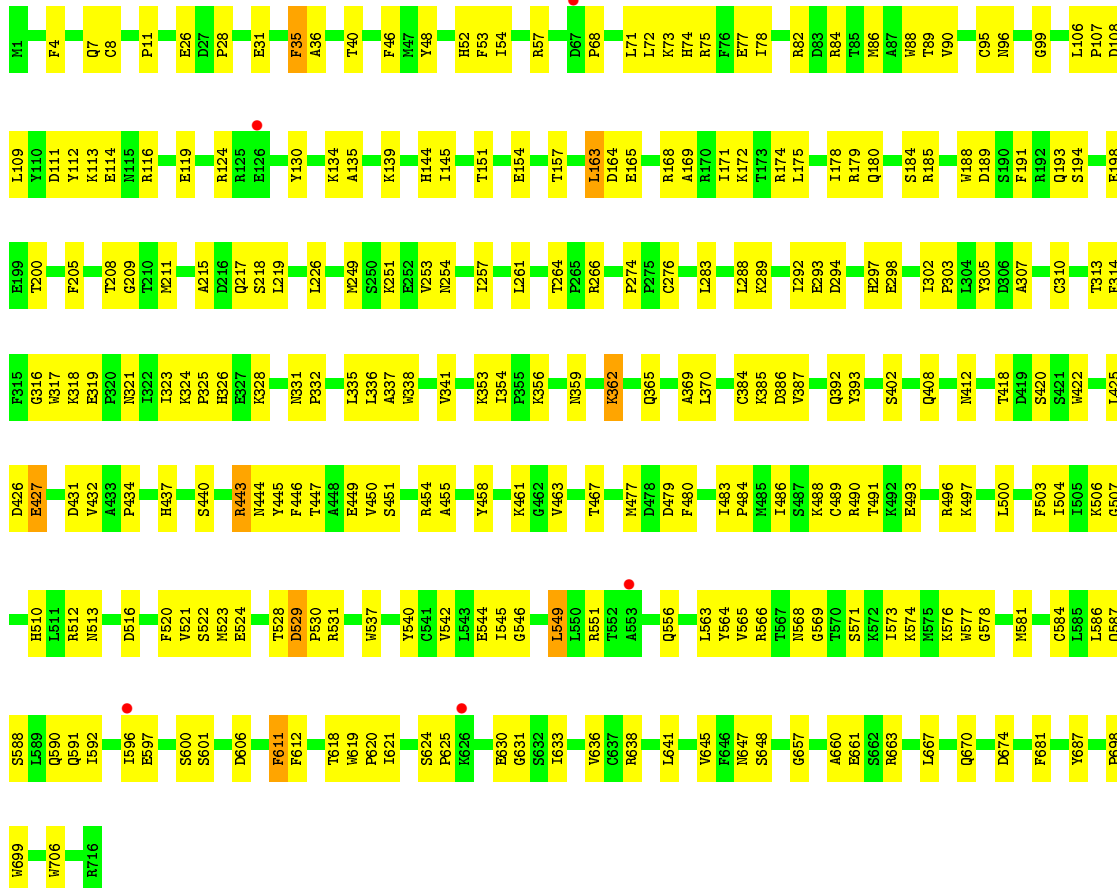


- Molecule 1: Polymerase acidic protein

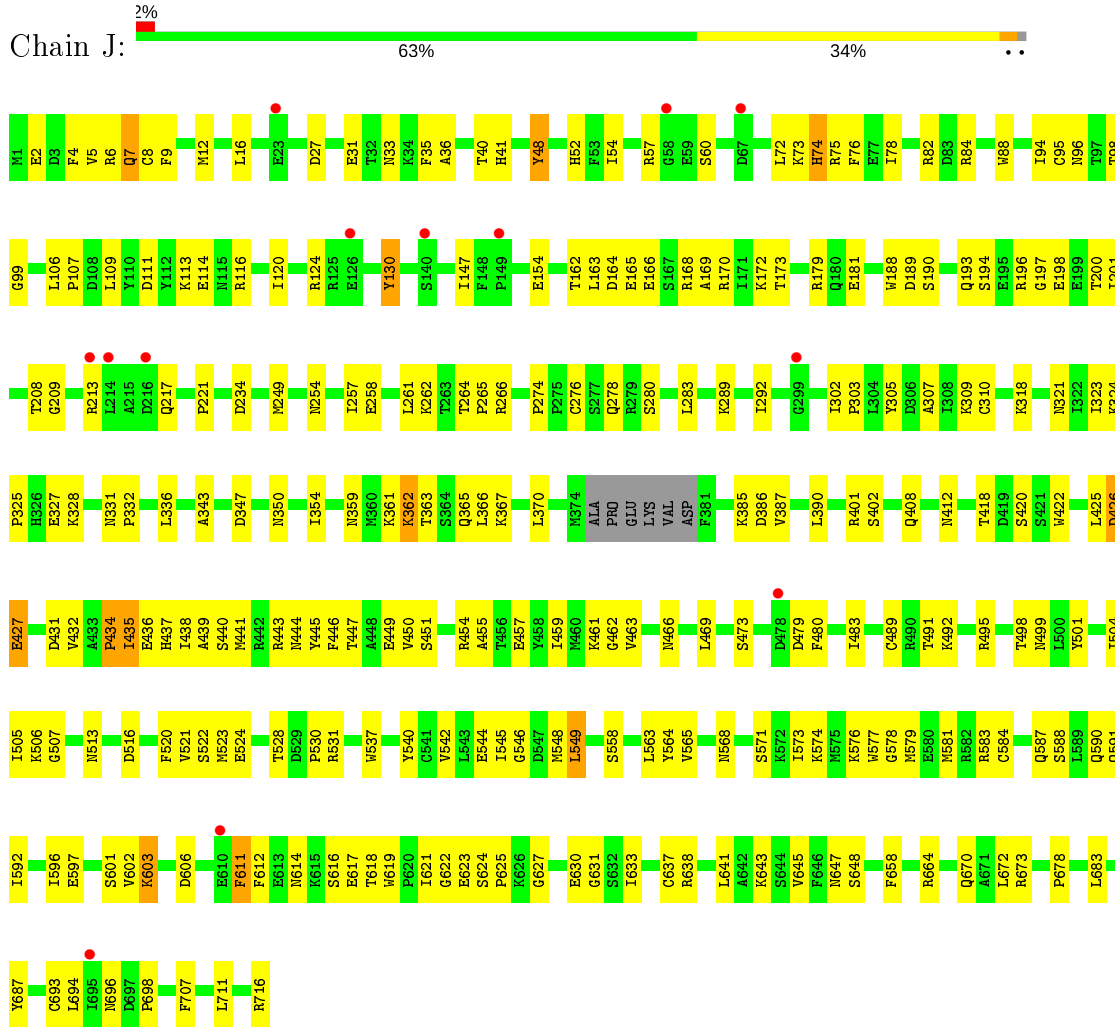




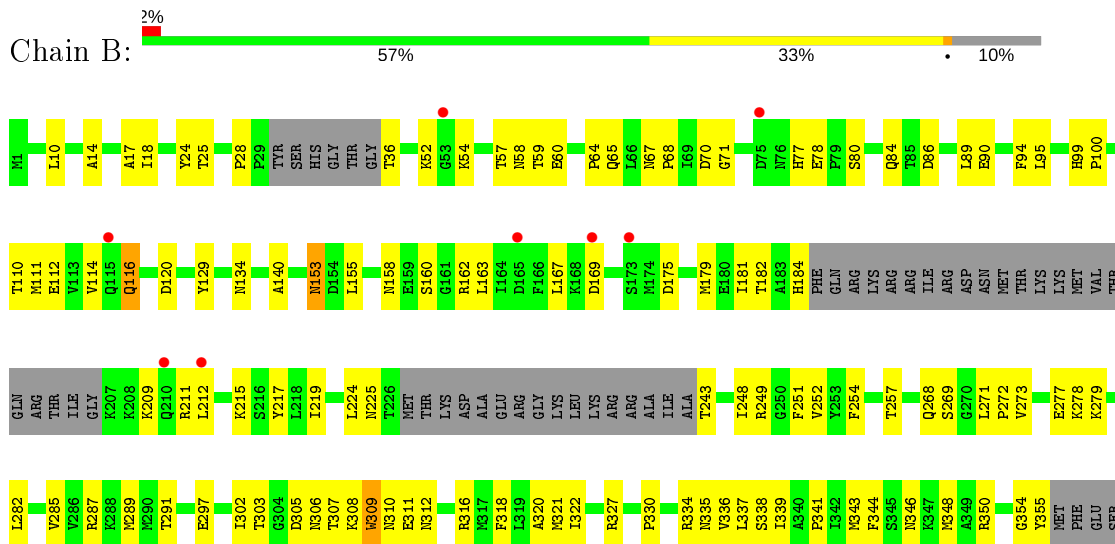
• Molecule 1: Polymerase acidic protein

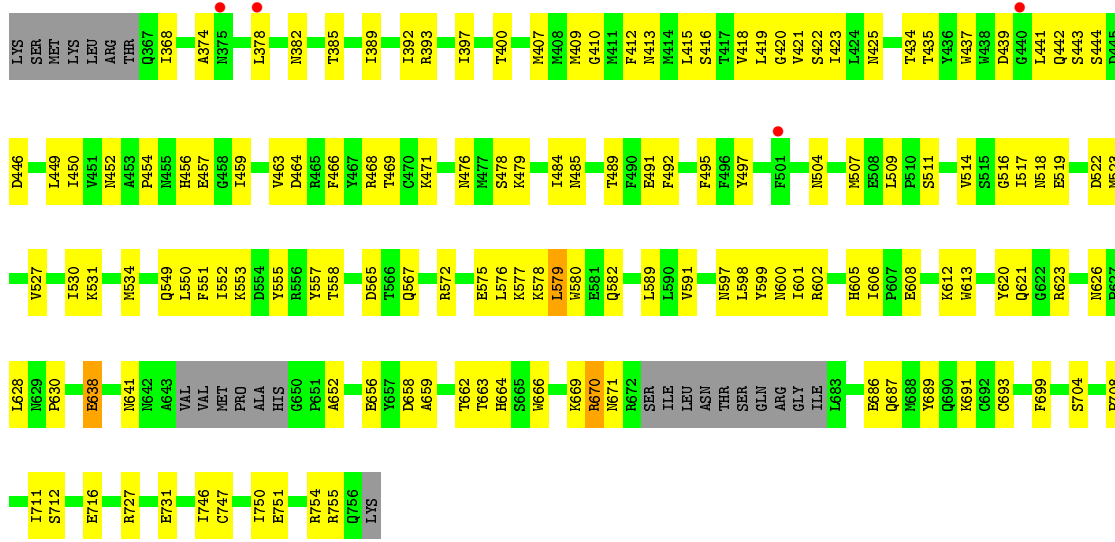


• Molecule 1: Polymerase acidic protein

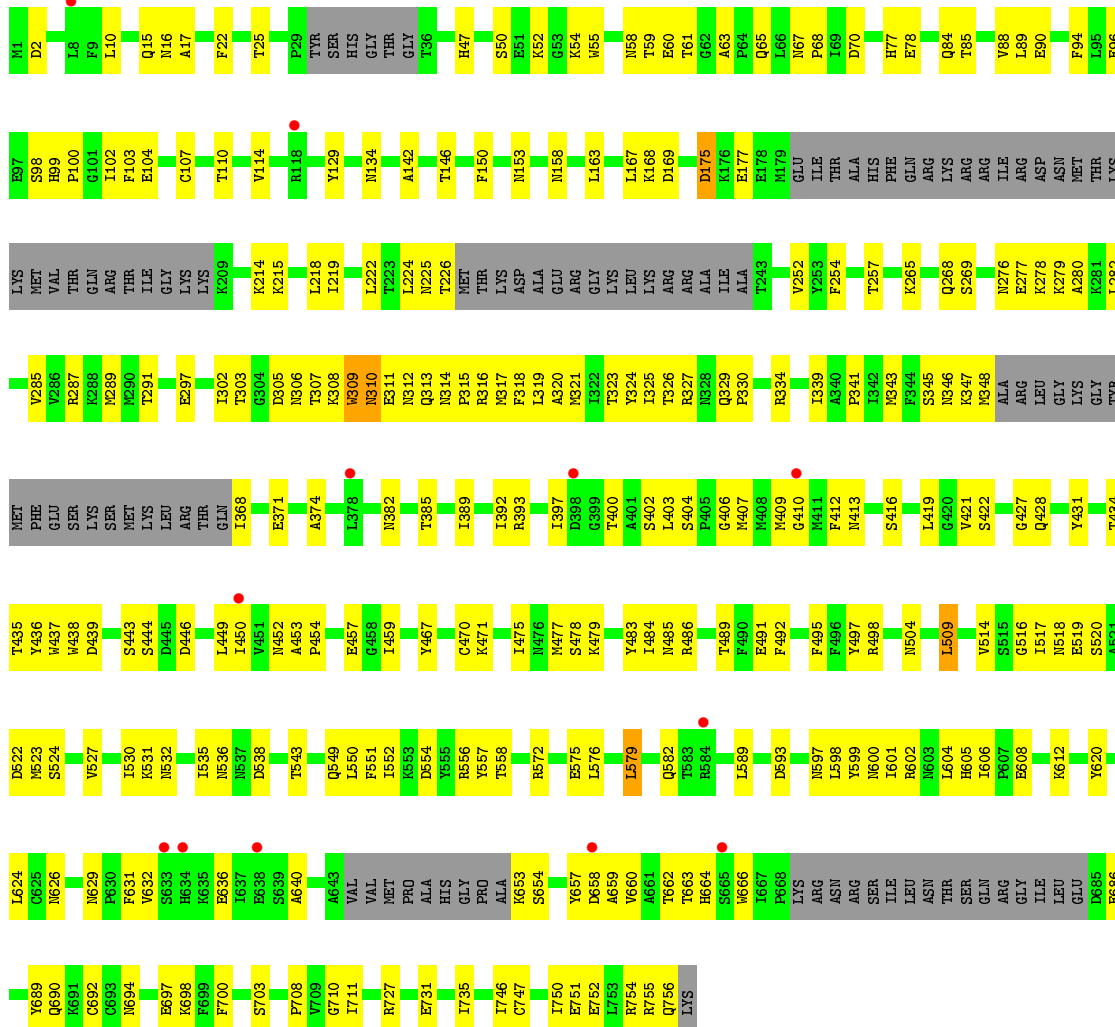


• Molecule 2: RNA-directed RNA polymerase catalytic subunit

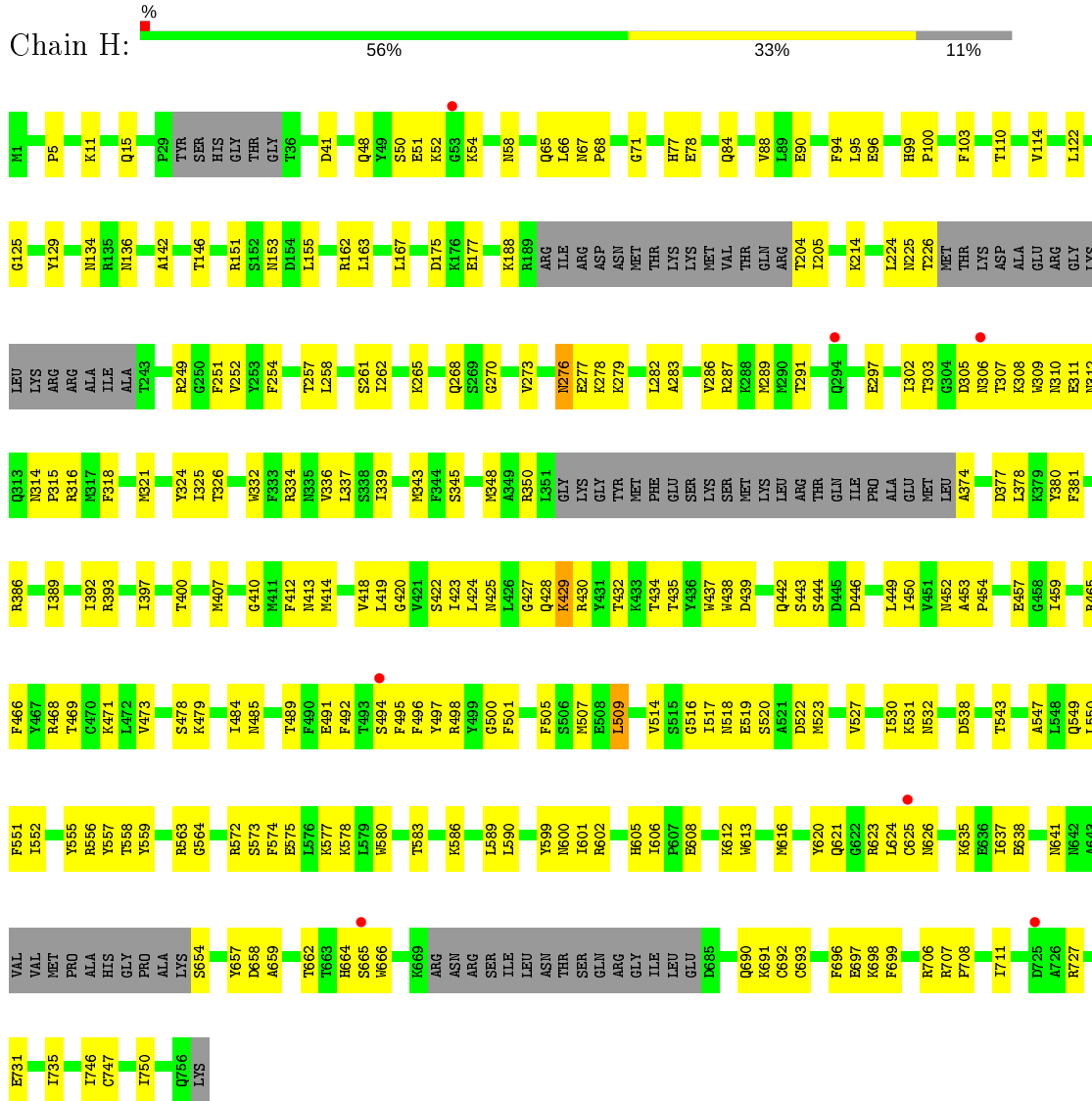




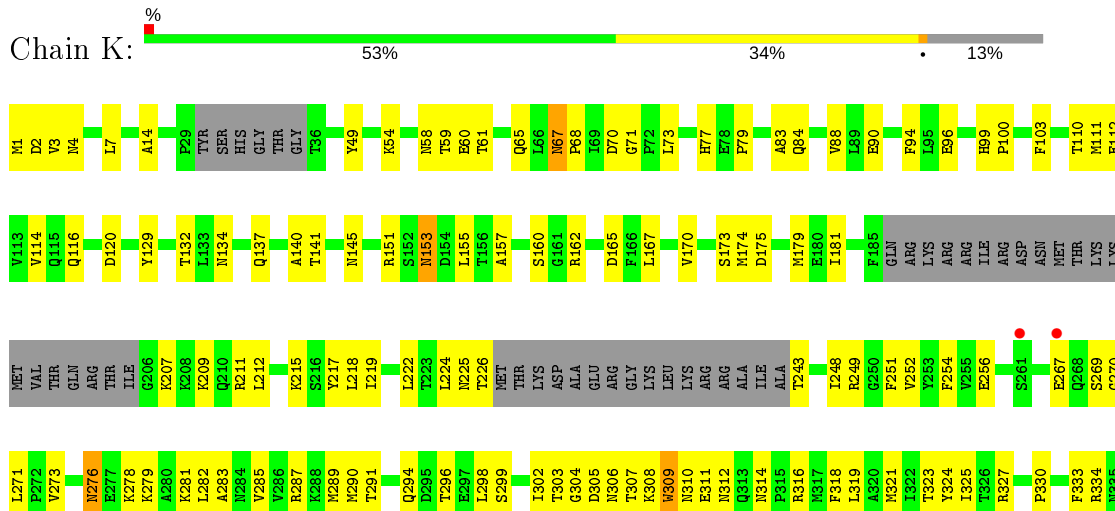
• Molecule 2: RNA-directed RNA polymerase catalytic subunit

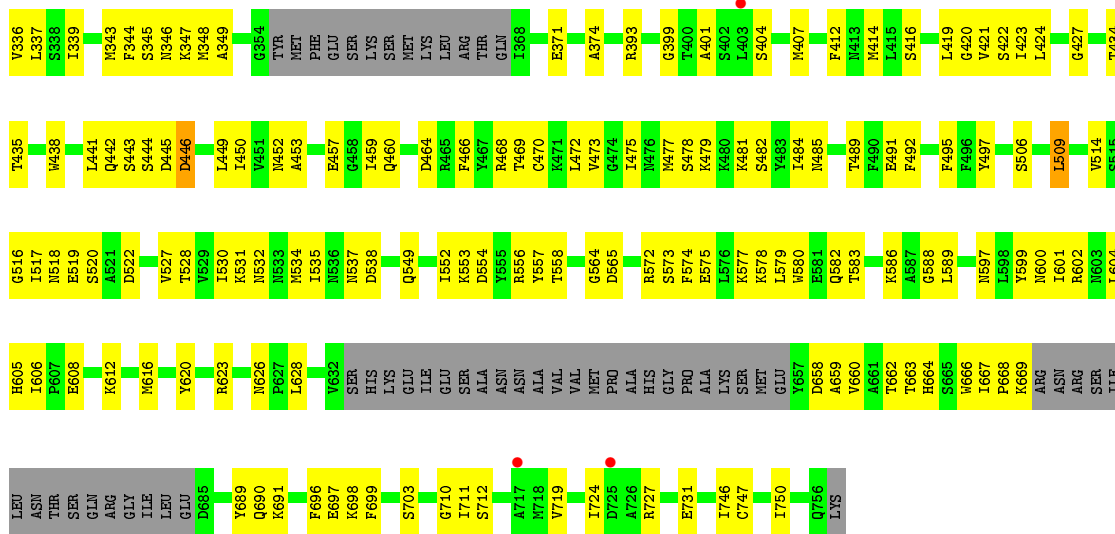


- Molecule 2: RNA-directed RNA polymerase catalytic subunit

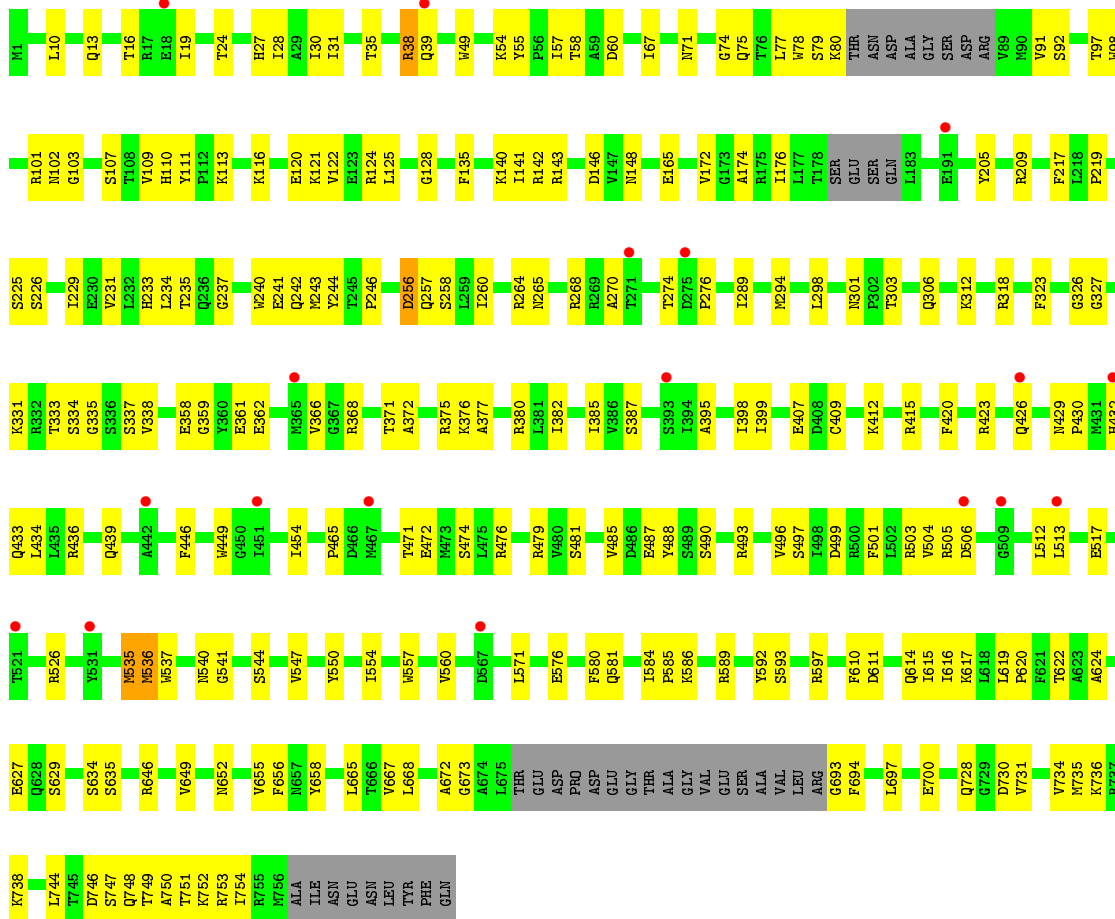


- Molecule 2: RNA-directed RNA polymerase catalytic subunit

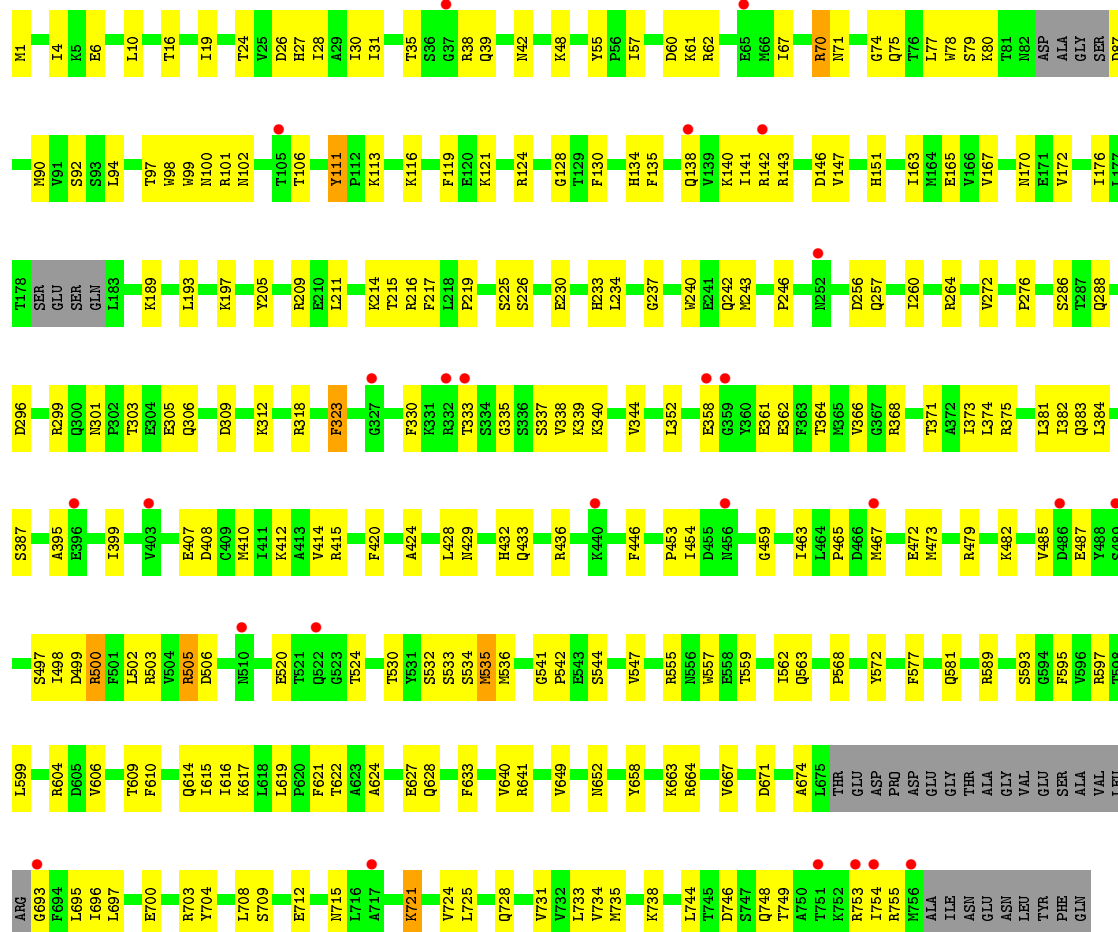




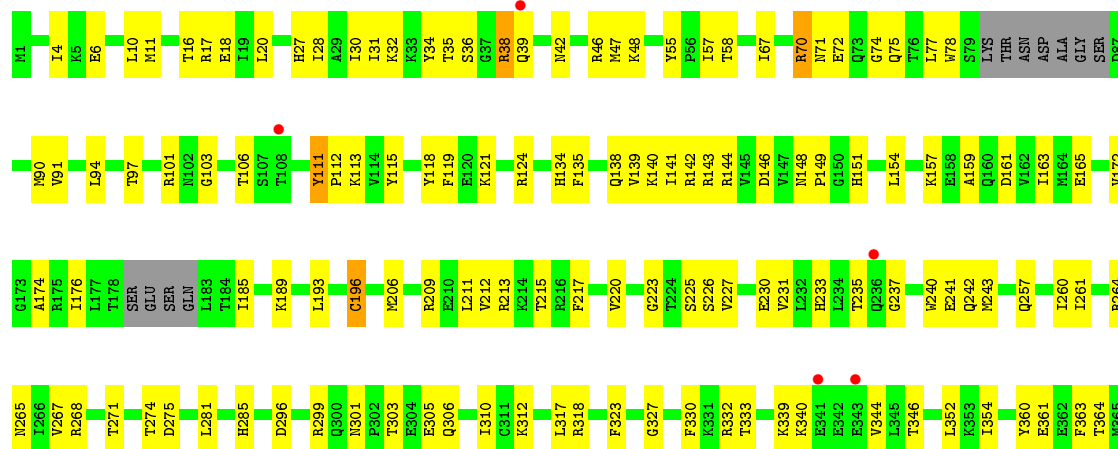
• Molecule 3: Polymerase basic protein 2

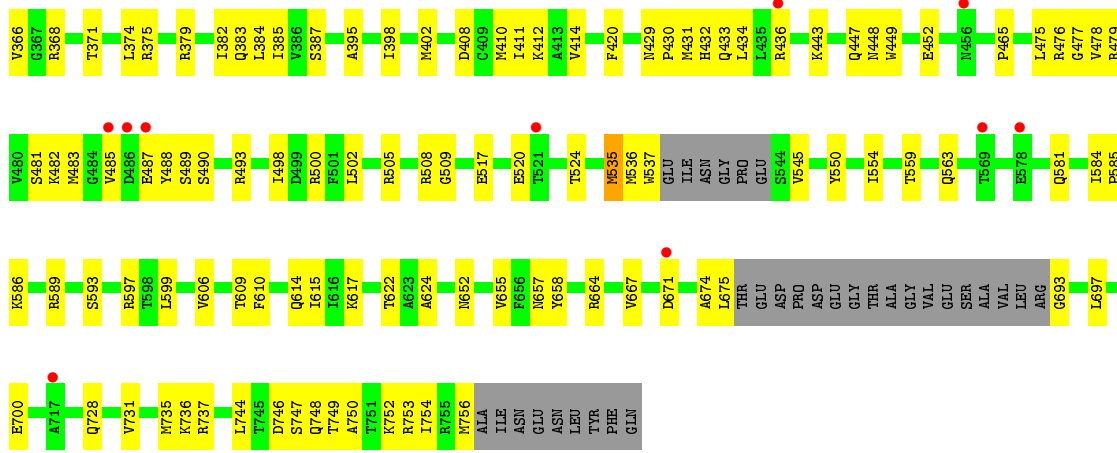


• Molecule 3: Polymerase basic protein 2

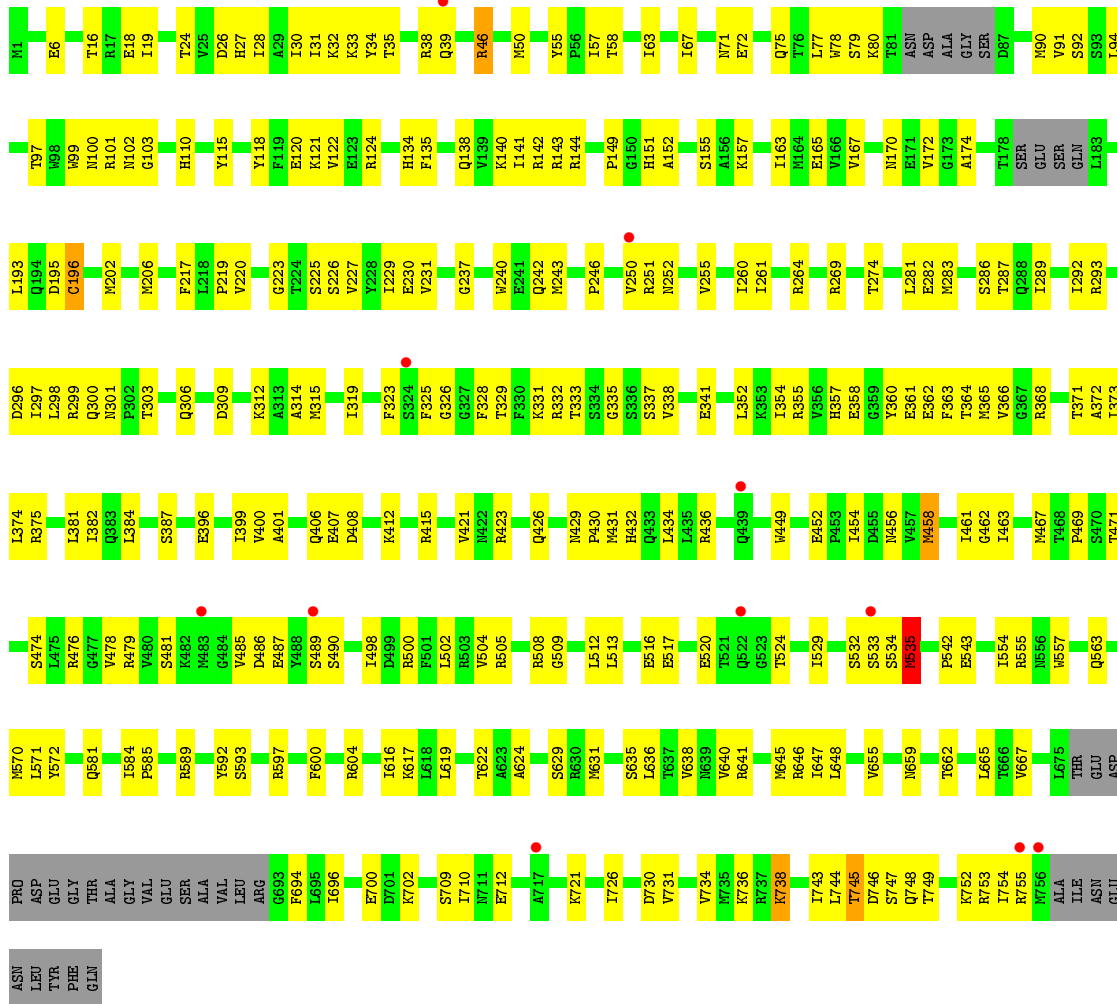


• Molecule 3: Polymerase basic protein 2





• Molecule 3: Polymerase basic protein 2



4 Data and refinement statistics i

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	337.12Å 192.86Å 235.69Å 90.00° 91.46° 90.00°	Depositor
Resolution (Å)	235.61 – 3.63 235.61 – 3.63	Depositor EDS
% Data completeness (in resolution range)	48.0 (235.61-3.63) 48.0 (235.61-3.63)	Depositor EDS
R_{merge}	0.48	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.31 (at 3.68Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.277 , 0.323 0.277 , 0.323	Depositor DCC
R_{free} test set	4059 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	76.8	Xtriage
Anisotropy	0.063	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 85.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.023 for -1/2*h-3/2*k,-1/2*h+1/2*k,-l 0.027 for -1/2*h+3/2*k,1/2*h+1/2*k,-l 0.026 for 1/2*h-3/2*k,-1/2*h-1/2*k,-l 0.035 for 1/2*h+3/2*k,1/2*h-1/2*k,-l 0.035 for -h,-k,l	Xtriage
F_o, F_c correlation	0.80	EDS
Total number of atoms	67760	wwPDB-VP
Average B, all atoms (Å ²)	101.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.59% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.27	0/5921	0.47	0/7981
1	D	0.26	0/5921	0.46	0/7981
1	G	0.27	0/5921	0.48	1/7981 (0.0%)
1	J	0.26	0/5874	0.46	0/7915
2	B	0.27	0/5580	0.47	0/7527
2	E	0.26	0/5386	0.45	0/7270
2	H	0.27	0/5493	0.47	0/7409
2	K	0.26	0/5394	0.46	0/7278
3	C	0.26	0/5883	0.48	0/7928
3	F	0.25	0/5917	0.48	0/7974
3	I	0.26	0/5846	0.49	0/7876
3	L	0.26	0/5909	0.49	0/7963
All	All	0.26	0/69045	0.47	1/93083 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	257	ILE	C-N-CA	-5.14	108.84	121.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	5796	0	5734	206	0
1	D	5796	0	5734	173	0
1	G	5796	0	5734	196	0
1	J	5751	0	5689	209	0
2	B	5474	0	5423	206	0
2	E	5283	0	5219	208	0
2	H	5389	0	5338	219	0
2	K	5290	0	5246	226	0
3	C	5790	0	5939	200	0
3	F	5824	0	5969	181	1
3	I	5755	0	5903	205	1
3	L	5816	0	5963	216	0
All	All	67760	0	67891	2181	1

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 16.

All (2181) 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)
3:I:318:ARG:HD3	3:I:493:ARG:HB3	1.54	0.90
1:G:321:ASN:HB3	1:G:544:GLU:HB3	1.52	0.89
1:G:68:PRO:HB3	1:G:72:LEU:HG	1.56	0.87
1:J:7:GLN:NE2	1:J:8:CYS:SG	2.48	0.87
2:H:485:ASN:ND2	2:H:489:THR:O	2.08	0.86
2:E:434:THR:HG22	2:E:435:THR:H	1.40	0.85
1:D:321:ASN:HB3	1:D:544:GLU:HB3	1.57	0.85
1:G:217:GLN:HE22	2:H:58:ASN:HA	1.42	0.85
2:H:527:VAL:HG21	2:H:599:TYR:HE2	1.41	0.84
1:J:321:ASN:HB3	1:J:544:GLU:HB3	1.60	0.84
1:A:190:SER:HB2	1:A:193:GLN:HE21	1.42	0.83
3:L:149:PRO:HB2	3:L:250:VAL:HG11	1.60	0.83
1:J:48:TYR:CE1	1:J:163:LEU:HD12	2.13	0.83
1:A:578:GLY:HA2	1:A:581:MET:HG3	1.59	0.83
3:C:148:ASN:ND2	3:C:209:ARG:O	2.12	0.83
2:B:308:LYS:O	2:B:312:ASN:ND2	2.12	0.83
2:H:302:ILE:HG22	2:H:484:ILE:HG23	1.59	0.83
2:B:485:ASN:ND2	2:B:489:THR:O	2.12	0.82
1:J:432:VAL:HG23	1:J:434:PRO:HD2	1.59	0.82
2:H:308:LYS:O	2:H:312:ASN:ND2	2.13	0.82
2:B:549:GLN:HA	2:B:552:ILE:HD12	1.61	0.81
1:J:189:ASP:HA	2:K:162:ARG:HH12	1.42	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:387:SER:HB3	3:I:481:SER:HB3	1.62	0.81
1:D:26:GLU:HG3	1:D:31:GLU:HG3	1.60	0.81
3:C:338:VAL:HB	3:C:358:GLU:HB3	1.63	0.80
3:C:614:GLN:NE2	3:C:649:VAL:O	2.14	0.80
2:E:302:ILE:HG22	2:E:484:ILE:HG23	1.63	0.80
2:H:177:GLU:HA	2:H:214:LYS:HB2	1.64	0.80
2:K:71:GLY:O	2:K:84:GLN:NE2	2.15	0.80
1:J:48:TYR:CE1	1:J:163:LEU:CD1	2.65	0.80
3:F:597:ARG:NH2	3:F:622:THR:O	2.15	0.79
3:F:362:GLU:HG3	3:F:375:ARG:HG2	1.62	0.79
2:B:613:TRP:O	2:B:621:GLN:NE2	2.15	0.79
2:E:177:GLU:HA	2:E:214:LYS:HB2	1.65	0.78
2:B:112:GLU:HG2	2:B:116:GLN:HE22	1.49	0.78
1:A:362:LYS:HG3	1:A:480:PHE:HE1	1.48	0.78
3:C:449:TRP:HE1	3:C:476:ARG:HB3	1.47	0.78
2:K:302:ILE:HG22	2:K:484:ILE:HG23	1.63	0.78
2:H:374:ALA:O	2:H:393:ARG:NH2	2.17	0.78
3:I:597:ARG:NH2	3:I:622:THR:O	2.17	0.77
2:B:269:SER:HB2	2:B:421:VAL:HG21	1.66	0.77
3:C:298:LEU:O	3:C:312:LYS:NZ	2.16	0.77
2:H:423:ILE:HD11	2:H:469:THR:HB	1.65	0.77
3:F:242:GLN:NE2	3:F:243:MET:O	2.18	0.77
2:H:564:GLY:HA2	2:H:577:LYS:HG2	1.64	0.77
1:G:75:ARG:NH1	1:G:111:ASP:OD2	2.17	0.77
1:D:449:GLU:O	1:D:638:ARG:NH2	2.19	0.76
1:G:477:MET:HG2	1:G:510:HIS:HD2	1.50	0.76
2:K:305:ASP:HB3	2:K:481:LYS:HB2	1.67	0.76
2:K:485:ASN:ND2	2:K:489:THR:O	2.18	0.76
2:B:129:TYR:OH	2:B:134:ASN:OD1	2.03	0.76
2:E:518:ASN:ND2	2:E:662:THR:O	2.19	0.76
3:I:275:ASP:HB3	1:J:96:ASN:HD21	1.50	0.76
2:K:307:THR:H	2:K:478:SER:HB2	1.50	0.76
2:K:153:ASN:ND2	2:K:179:MET:SD	2.58	0.76
3:L:387:SER:HB3	3:L:481:SER:HB3	1.68	0.76
1:G:392:GLN:HB2	2:H:381:PHE:HA	1.67	0.75
3:C:501:PHE:HZ	1:D:93:SER:HA	1.52	0.75
1:D:154:GLU:OE2	1:D:172:LYS:NZ	2.14	0.75
2:B:153:ASN:ND2	2:B:179:MET:SD	2.59	0.75
1:G:576:LYS:NZ	3:I:42:ASN:OD1	2.19	0.75
1:A:58:GLY:H	3:F:628:GLN:H	1.32	0.75
1:D:618:THR:HB	1:D:630:GLU:HB3	1.69	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:257:GLN:NE2	3:I:524:THR:O	2.20	0.74
3:I:746:ASP:O	3:I:749:THR:OG1	2.04	0.74
2:K:287:ARG:NH2	3:L:458:MET:O	2.19	0.74
1:D:530:PRO:HG3	1:D:542:VAL:HG11	1.69	0.74
1:G:408:GLN:O	1:G:412:ASN:ND2	2.20	0.74
3:C:697:LEU:HD11	3:C:735:MET:HB2	1.69	0.74
1:D:190:SER:HB2	1:D:193:GLN:HE21	1.51	0.74
1:G:54:ILE:HG13	1:G:75:ARG:HB2	1.70	0.74
1:A:408:GLN:O	1:A:412:ASN:ND2	2.21	0.74
3:L:745:THR:O	3:L:749:THR:N	2.20	0.74
3:F:700:GLU:HB2	3:F:731:VAL:HB	1.70	0.73
1:G:249:MET:HB3	2:H:468:ARG:HH21	1.53	0.73
2:H:95:LEU:HD12	2:H:422:SER:HA	1.70	0.73
1:J:106:LEU:HD22	1:J:107:PRO:O	1.87	0.73
1:J:234:ASP:O	2:K:327:ARG:NH2	2.21	0.73
2:H:637:ILE:HG13	2:H:638:GLU:HG2	1.71	0.73
3:I:449:TRP:HE1	3:I:476:ARG:HB3	1.53	0.73
1:D:359:ASN:ND2	1:D:479:ASP:OD2	2.22	0.72
1:J:217:GLN:HE22	2:K:58:ASN:HA	1.53	0.72
3:L:354:ILE:HD11	3:L:431:MET:HG2	1.72	0.72
3:L:289:ILE:HG13	3:L:529:ILE:HG23	1.71	0.72
3:C:499:ASP:HB3	3:C:505:ARG:HH12	1.54	0.72
3:L:332:ARG:NH2	3:L:361:GLU:OE2	2.23	0.72
1:J:408:GLN:O	1:J:412:ASN:ND2	2.21	0.72
1:A:530:PRO:HG3	1:A:542:VAL:HG11	1.72	0.72
1:D:469:LEU:HG	1:D:483:ILE:HD13	1.72	0.72
2:H:129:TYR:OH	2:H:134:ASN:OD1	2.07	0.72
2:E:65:GLN:NE2	2:E:345:SER:O	2.22	0.72
2:K:276:ASN:HB2	3:L:219:PRO:HG3	1.72	0.72
2:K:307:THR:N	2:K:478:SER:HB2	2.04	0.72
3:L:542:PRO:HG2	3:L:641:ARG:H	1.55	0.72
3:L:572:TYR:OH	3:L:604:ARG:NH2	2.22	0.71
1:D:122:VAL:HG22	1:D:148:PHE:HB2	1.73	0.71
2:H:599:TYR:OH	2:H:608:GLU:N	2.24	0.71
3:I:242:GLN:NE2	3:I:243:MET:O	2.23	0.71
2:K:103:PHE:HB3	2:K:325:ILE:HG23	1.72	0.71
3:L:436:ARG:NH2	3:L:516:GLU:O	2.23	0.71
2:E:307:THR:H	2:E:478:SER:HB2	1.55	0.71
3:F:10:LEU:O	3:F:16:THR:OG1	2.07	0.71
2:B:179:MET:HB3	2:B:212:LEU:HD23	1.72	0.71
1:D:612:PHE:HE1	1:D:633:ILE:HG21	1.56	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:562:ILE:HD12	3:F:563:GLN:N	2.05	0.71
1:G:8:CYS:O	1:G:174:ARG:NH2	2.24	0.71
3:I:148:ASN:ND2	3:I:209:ARG:O	2.22	0.71
1:A:3:ASP:OD1	3:C:318:ARG:NE	2.23	0.71
1:A:31:GLU:OE1	1:A:200:THR:OG1	2.08	0.71
2:B:423:ILE:HD11	2:B:469:THR:HB	1.72	0.71
2:E:489:THR:HA	2:E:497:TYR:O	1.91	0.71
1:J:124:ARG:NH1	1:J:194:SER:OG	2.22	0.71
1:G:266:ARG:O	1:G:687:TYR:OH	2.08	0.70
2:B:608:GLU:OE2	2:B:612:LYS:NZ	2.22	0.70
1:G:193:GLN:N	1:G:193:GLN:OE1	2.24	0.70
2:E:708:PRO:HB3	3:F:728:GLN:HG3	1.73	0.70
2:K:308:LYS:O	2:K:312:ASN:ND2	2.25	0.70
1:A:321:ASN:HB3	1:A:544:GLU:HB3	1.72	0.70
2:B:268:GLN:NE2	2:B:439:ASP:OD1	2.24	0.70
2:H:270:GLY:O	2:H:278:LYS:NZ	2.24	0.70
2:E:129:TYR:OH	2:E:134:ASN:OD1	2.09	0.70
1:A:276:CYS:HB2	1:A:698:PRO:HG3	1.74	0.69
1:A:714:ALA:HA	2:B:10:LEU:HD21	1.74	0.69
2:H:279:LYS:HA	2:H:282:LEU:HD12	1.74	0.69
1:A:432:VAL:HG23	1:A:434:PRO:HD2	1.73	0.69
2:B:302:ILE:HG22	2:B:484:ILE:HG23	1.74	0.69
2:H:15:GLN:OE1	2:H:498:ARG:NH2	2.22	0.69
2:H:489:THR:HA	2:H:497:TYR:O	1.93	0.69
2:H:573:SER:HB3	2:H:577:LYS:HE3	1.73	0.69
3:L:71:ASN:ND2	3:L:75:GLN:OE1	2.25	0.69
3:F:296:ASP:OD1	3:F:299:ARG:NH1	2.25	0.69
2:H:310:ASN:ND2	2:H:407:MET:O	2.25	0.69
3:I:700:GLU:HB2	3:I:731:VAL:HB	1.72	0.69
1:D:408:GLN:O	1:D:412:ASN:ND2	2.24	0.69
1:J:193:GLN:OE1	1:J:193:GLN:N	2.25	0.69
1:G:336:LEU:HD23	1:G:365:GLN:HE21	1.58	0.69
1:A:324:LYS:NZ	1:A:325:PRO:O	2.22	0.69
3:I:420:PHE:O	3:I:433:GLN:NE2	2.26	0.69
1:J:106:LEU:CD2	1:J:107:PRO:O	2.40	0.69
2:K:88:VAL:HG22	2:K:473:VAL:HG12	1.74	0.69
2:B:287:ARG:O	2:B:291:THR:OG1	2.10	0.69
3:C:71:ASN:ND2	3:C:75:GLN:OE1	2.26	0.69
3:I:597:ARG:NH2	3:I:624:ALA:O	2.26	0.69
3:I:697:LEU:HD11	3:I:735:MET:HB2	1.75	0.69
2:K:573:SER:HB3	2:K:577:LYS:HE3	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:323:ILE:HD11	1:A:544:GLU:HB2	1.73	0.69
3:F:121:LYS:HA	3:F:124:ARG:HD2	1.75	0.69
3:F:55:TYR:HE1	3:F:77:LEU:HA	1.58	0.69
2:E:434:THR:HG22	2:E:435:THR:N	2.07	0.68
3:I:261:ILE:HD13	3:I:524:THR:H	1.58	0.68
2:K:518:ASN:ND2	2:K:662:THR:O	2.27	0.68
3:L:57:ILE:HB	3:L:91:VAL:O	1.94	0.68
2:B:297:GLU:OE2	2:B:437:TRP:NE1	2.24	0.68
3:C:387:SER:HB3	3:C:481:SER:HB3	1.76	0.68
1:D:124:ARG:NH1	1:D:194:SER:OG	2.26	0.68
2:H:291:THR:O	3:I:383:GLN:NE2	2.24	0.68
2:B:489:THR:HA	2:B:497:TYR:O	1.93	0.68
1:J:336:LEU:HD23	1:J:365:GLN:HE21	1.57	0.68
2:K:527:VAL:HG21	2:K:599:TYR:HE2	1.56	0.68
2:B:71:GLY:O	2:B:84:GLN:NE2	2.27	0.68
2:E:347:LYS:NZ	2:E:403:LEU:O	2.26	0.68
3:I:652:ASN:OD1	3:I:658:TYR:N	2.24	0.68
1:J:506:LYS:NZ	1:J:507:GLY:O	2.21	0.68
3:L:505:ARG:NH1	3:L:509:GLY:O	2.25	0.68
2:E:453:ALA:HB3	2:E:459:ILE:HG12	1.75	0.68
1:J:78:ILE:HA	1:J:109:LEU:HD12	1.76	0.68
2:K:181:ILE:HD11	2:K:212:LEU:HB2	1.75	0.68
3:C:121:LYS:HA	3:C:124:ARG:HD2	1.76	0.68
3:F:420:PHE:O	3:F:433:GLN:NE2	2.26	0.68
3:F:532:SER:OG	3:F:555:ARG:NH1	2.20	0.68
2:H:71:GLY:O	2:H:84:GLN:NE2	2.27	0.67
3:L:478:VAL:O	3:L:479:ARG:NH1	2.26	0.67
2:E:549:GLN:HA	2:E:552:ILE:HD12	1.75	0.67
1:A:362:LYS:HG3	1:A:480:PHE:CE1	2.29	0.67
1:D:283:LEU:O	1:D:461:LYS:NZ	2.26	0.67
1:G:647:ASN:OD1	1:G:699:TRP:NE1	2.22	0.67
1:J:693:CYS:O	1:J:694:LEU:HD12	1.94	0.67
2:K:423:ILE:HD11	2:K:469:THR:HB	1.76	0.67
1:A:427:GLU:O	2:B:597:ASN:ND2	2.28	0.67
1:A:449:GLU:O	1:A:638:ARG:NH2	2.28	0.67
2:E:485:ASN:ND2	2:E:489:THR:O	2.26	0.67
1:G:324:LYS:NZ	1:G:325:PRO:O	2.23	0.67
3:I:366:VAL:HA	3:I:371:THR:HG22	1.77	0.67
3:L:326:GLY:N	3:L:517:GLU:OE1	2.28	0.67
3:L:387:SER:OG	3:L:485:VAL:N	2.28	0.67
2:H:434:THR:HG22	2:H:435:THR:H	1.59	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:527:VAL:HG21	2:H:599:TYR:CE2	2.27	0.67
3:L:242:GLN:NE2	3:L:243:MET:O	2.27	0.67
2:E:657:TYR:OH	3:F:209:ARG:NH2	2.27	0.67
3:F:497:SER:OG	3:F:505:ARG:O	2.11	0.67
1:A:447:THR:O	1:A:451:SER:N	2.26	0.67
3:F:338:VAL:HB	3:F:358:GLU:HB3	1.77	0.67
3:C:101:ARG:NE	3:C:102:ASN:OD1	2.24	0.67
3:C:256:ASP:OD2	3:C:301:ASN:ND2	2.20	0.67
1:D:118:ILE:HG12	1:D:144:HIS:HB3	1.77	0.67
1:D:506:LYS:NZ	1:D:507:GLY:O	2.21	0.67
3:I:387:SER:OG	3:I:485:VAL:N	2.27	0.67
2:K:289:MET:O	2:K:452:ASN:ND2	2.28	0.67
2:E:517:ILE:N	2:E:522:ASP:OD2	2.24	0.66
1:G:432:VAL:HG23	1:G:434:PRO:HD2	1.76	0.66
2:B:297:GLU:HA	2:B:454:PRO:HA	1.77	0.66
2:K:279:LYS:HA	2:K:282:LEU:HD12	1.77	0.66
2:H:291:THR:OG1	3:I:383:GLN:OE1	2.14	0.66
2:K:252:VAL:HG23	2:K:412:PHE:HE1	1.61	0.66
3:C:242:GLN:NE2	3:C:243:MET:O	2.29	0.66
1:J:624:SER:HB3	2:K:1:MET:HA	1.77	0.66
3:L:298:LEU:O	3:L:312:LYS:NZ	2.28	0.66
1:D:125:ARG:HD3	1:D:195:GLU:HG3	1.76	0.66
3:F:71:ASN:ND2	3:F:75:GLN:OE1	2.28	0.66
1:G:447:THR:O	1:G:451:SER:N	2.29	0.66
1:G:321:ASN:ND2	1:G:544:GLU:OE1	2.29	0.66
3:L:352:LEU:HD13	3:L:430:PRO:HB3	1.76	0.66
1:D:362:LYS:HG3	1:D:480:PHE:HE1	1.60	0.66
1:G:427:GLU:OE1	2:H:563:ARG:NH1	2.29	0.66
3:L:597:ARG:NH2	3:L:624:ALA:O	2.29	0.66
3:I:498:ILE:HD11	3:I:502:LEU:HA	1.77	0.66
1:A:387:VAL:HB	1:A:390:LEU:HB2	1.77	0.66
1:D:500:LEU:HD21	1:D:503:PHE:HE1	1.61	0.66
2:H:613:TRP:O	2:H:621:GLN:NE2	2.27	0.66
3:C:446:PHE:HB2	3:C:465:PRO:HB3	1.78	0.66
2:E:593:ASP:OD2	3:F:100:ASN:ND2	2.29	0.66
1:J:198:GLU:HG2	1:J:200:THR:HG22	1.77	0.66
1:G:254:ASN:O	2:H:77:HIS:NE2	2.29	0.66
1:J:530:PRO:HG3	1:J:542:VAL:HG11	1.78	0.66
3:C:257:GLN:NE2	3:C:258:SER:OG	2.29	0.65
1:J:54:ILE:HG13	1:J:75:ARG:HB2	1.78	0.65
3:L:449:TRP:HE1	3:L:476:ARG:HB3	1.61	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:549:GLN:HA	2:H:552:ILE:HD12	1.77	0.65
3:C:560:VAL:HG13	3:C:571:LEU:HD11	1.78	0.65
3:C:597:ARG:NH2	3:C:624:ALA:O	2.29	0.65
2:H:78:GLU:O	2:H:471:LYS:NZ	2.30	0.65
3:I:753:ARG:NH1	3:I:756:MET:SD	2.69	0.65
1:J:154:GLU:OE2	1:J:168:ARG:NH1	2.29	0.65
3:I:332:ARG:NH2	3:I:361:GLU:OE2	2.29	0.65
1:J:447:THR:O	1:J:451:SER:N	2.29	0.65
1:J:597:GLU:O	1:J:601:SER:N	2.30	0.65
2:E:751:GLU:OE2	2:E:755:ARG:NH2	2.29	0.65
1:G:578:GLY:HA2	1:G:581:MET:HG3	1.78	0.65
1:G:359:ASN:ND2	1:G:479:ASP:OD2	2.30	0.65
2:K:54:LYS:HG3	2:K:68:PRO:HA	1.79	0.65
1:A:261:LEU:O	1:A:264:THR:OG1	2.14	0.65
1:A:205:PHE:O	2:B:335:ASN:ND2	2.29	0.65
2:E:309:TRP:O	2:E:313:GLN:NE2	2.29	0.65
2:E:710:GLY:N	3:F:26:ASP:OD1	2.27	0.65
2:H:224:LEU:O	2:H:350:ARG:N	2.26	0.65
2:H:273:VAL:HB	2:H:277:GLU:HG3	1.77	0.64
2:H:311:GLU:OE1	2:H:311:GLU:N	2.29	0.64
1:J:462:GLY:O	1:J:466:ASN:ND2	2.29	0.64
3:L:165:GLU:HG2	3:L:172:VAL:HG21	1.78	0.64
1:G:185:ARG:HE	3:I:157:LYS:HE2	1.62	0.64
1:J:266:ARG:O	1:J:687:TYR:OH	2.14	0.64
1:J:449:GLU:O	1:J:638:ARG:NH2	2.27	0.64
2:B:355:TYR:HB2	2:B:368:ILE:HD11	1.79	0.64
2:E:311:GLU:OE1	2:E:311:GLU:N	2.30	0.64
2:E:308:LYS:O	2:E:312:ASN:ND2	2.30	0.64
1:G:164:ASP:OD1	1:G:165:GLU:N	2.31	0.64
3:C:593:SER:HB2	3:C:624:ALA:HB3	1.77	0.64
3:F:581:GLN:OE1	3:F:589:ARG:NH1	2.30	0.64
2:E:518:ASN:N	2:E:522:ASP:OD2	2.30	0.64
2:E:605:HIS:HB3	3:F:233:HIS:HE1	1.62	0.64
2:H:608:GLU:OE2	2:H:612:LYS:NZ	2.22	0.64
1:D:266:ARG:HB2	1:D:687:TYR:HE2	1.61	0.64
3:L:384:LEU:O	3:L:479:ARG:N	2.30	0.64
1:A:24:TYR:OH	1:A:84:ARG:NH1	2.31	0.64
3:C:366:VAL:HA	3:C:371:THR:HG22	1.79	0.64
2:E:690:GLN:O	2:E:694:ASN:ND2	2.20	0.64
3:F:101:ARG:NE	3:F:102:ASN:OD1	2.22	0.64
3:L:337:SER:OG	3:L:361:GLU:OE2	2.13	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:514:VAL:HG11	2:B:558:THR:HG21	1.80	0.64
1:G:612:PHE:HE1	1:G:633:ILE:HG21	1.62	0.64
3:L:309:ASP:HB3	3:L:319:ILE:HD13	1.78	0.64
3:C:10:LEU:O	3:C:16:THR:OG1	2.09	0.64
2:B:374:ALA:O	2:B:393:ARG:NH2	2.31	0.64
1:G:606:ASP:HB2	3:I:135:PHE:CG	2.32	0.64
2:H:103:PHE:HB3	2:H:325:ILE:HG23	1.79	0.64
1:G:189:ASP:HA	2:H:162:ARG:HH12	1.63	0.64
1:A:670:GLN:HG2	2:B:14:ALA:H	1.63	0.63
2:E:276:ASN:ND2	2:E:538:ASP:OD1	2.31	0.63
1:G:463:VAL:O	1:G:467:THR:OG1	2.14	0.63
2:H:578:LYS:NZ	3:I:72:GLU:OE2	2.24	0.63
3:L:155:SER:HB3	3:L:300:GLN:HB3	1.80	0.63
1:A:36:ALA:O	1:A:40:THR:OG1	2.16	0.63
1:J:173:THR:OG1	3:L:696:ILE:N	2.23	0.63
1:J:359:ASN:ND2	1:J:479:ASP:OD2	2.30	0.63
2:K:527:VAL:HA	2:K:530:ILE:HD12	1.80	0.63
1:A:596:ILE:O	1:A:600:SER:OG	2.13	0.63
3:F:697:LEU:HD11	3:F:735:MET:HB2	1.80	0.63
2:H:708:PRO:HA	3:I:728:GLN:HE21	1.62	0.63
3:C:597:ARG:NH2	3:C:622:THR:O	2.31	0.63
1:D:420:SER:HB3	1:D:489:CYS:HB2	1.79	0.63
3:F:748:GLN:N	3:F:748:GLN:OE1	2.29	0.63
2:H:708:PRO:HB3	3:I:728:GLN:HG3	1.80	0.63
3:C:744:LEU:HD12	3:C:746:ASP:H	1.64	0.63
3:F:135:PHE:CZ	3:F:240:TRP:HB3	2.33	0.63
1:G:551:ARG:HA	1:G:556:GLN:HA	1.81	0.63
1:J:324:LYS:NZ	1:J:325:PRO:O	2.31	0.63
2:K:606:ILE:HD13	3:L:122:VAL:HG22	1.79	0.63
2:K:572:ARG:NH2	3:L:97:THR:OG1	2.28	0.63
2:E:747:CYS:HA	2:E:750:ILE:HD12	1.81	0.63
3:F:124:ARG:NH1	3:F:230:GLU:OE1	2.32	0.63
2:H:153:ASN:HB2	2:H:155:LEU:HD12	1.81	0.63
3:I:165:GLU:HG2	3:I:172:VAL:HG21	1.81	0.63
3:L:557:TRP:CE3	3:L:616:ILE:HD11	2.34	0.63
1:G:362:LYS:HG3	1:G:480:PHE:HE1	1.64	0.63
2:H:563:ARG:HH21	2:H:580:TRP:HH2	1.47	0.63
1:J:324:LYS:HZ1	1:J:327:GLU:HG3	1.63	0.63
2:E:158:ASN:N	2:E:169:ASP:OD2	2.32	0.62
3:F:142:ARG:HB3	3:F:217:PHE:CE1	2.34	0.62
2:H:276:ASN:ND2	2:H:538:ASP:OD1	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:302:ILE:HD12	1:J:303:PRO:HD2	1.80	0.62
1:J:48:TYR:HE1	1:J:163:LEU:CD1	2.12	0.62
1:G:84:ARG:HE	1:G:88:TRP:HE1	1.45	0.62
1:J:164:ASP:OD1	1:J:165:GLU:N	2.32	0.62
2:K:588:GLY:HA2	2:K:612:LYS:HB3	1.81	0.62
1:A:54:ILE:HG13	1:A:75:ARG:HB2	1.82	0.62
1:A:647:ASN:OD1	1:A:699:TRP:NE1	2.32	0.62
3:C:335:GLY:HA3	3:C:361:GLU:HA	1.81	0.62
2:E:608:GLU:OE2	2:E:612:LYS:NZ	2.31	0.62
1:G:621:ILE:HD11	1:G:631:GLY:HA3	1.82	0.62
1:A:483:ILE:HD11	1:A:506:LYS:HB2	1.81	0.62
3:I:124:ARG:NH1	3:I:230:GLU:OE1	2.30	0.62
2:K:276:ASN:ND2	2:K:538:ASP:OD1	2.32	0.62
2:H:307:THR:N	2:H:478:SER:HB2	2.14	0.62
3:C:499:ASP:OD2	3:C:505:ARG:NH2	2.32	0.62
1:D:432:VAL:HG23	1:D:434:PRO:HD2	1.82	0.62
2:H:377:ASP:HB3	2:H:380:TYR:HE2	1.64	0.62
2:H:708:PRO:HB3	3:I:728:GLN:HE21	1.63	0.62
2:K:719:VAL:HG13	2:K:747:CYS:HB3	1.82	0.62
2:B:516:GLY:N	2:B:522:ASP:OD1	2.32	0.62
3:C:504:VAL:HG12	3:C:512:LEU:HD12	1.80	0.62
1:G:323:ILE:HG23	1:G:531:ARG:HH21	1.65	0.62
1:J:435:ILE:O	1:J:439:ALA:N	2.26	0.62
2:K:492:PHE:O	2:K:495:PHE:HB2	1.99	0.62
3:C:535:MET:HG2	3:C:536:MET:H	1.64	0.62
3:C:554:ILE:HD11	3:C:665:LEU:HD23	1.82	0.62
1:D:590:GLN:HB3	2:E:543:THR:HG21	1.82	0.62
2:K:285:VAL:HG21	2:K:441:LEU:HD11	1.80	0.62
1:A:208:THR:HG22	1:A:209:GLY:H	1.64	0.62
2:H:590:LEU:HA	2:H:612:LYS:HZ2	1.65	0.62
2:E:276:ASN:ND2	2:E:535:ILE:O	2.30	0.61
2:E:520:SER:HB3	2:E:662:THR:HG21	1.82	0.61
2:H:378:LEU:HB3	2:H:386:ARG:HG3	1.81	0.61
2:H:575:GLU:OE2	3:I:101:ARG:NH1	2.33	0.61
3:I:71:ASN:ND2	3:I:75:GLN:OE1	2.33	0.61
1:J:292:ILE:HD11	1:J:310:CYS:SG	2.40	0.61
1:J:265:PRO:O	1:J:716:ARG:NH2	2.33	0.61
3:F:412:LYS:O	3:F:415:ARG:NH1	2.31	0.61
3:I:352:LEU:HD13	3:I:430:PRO:HB3	1.82	0.61
3:I:420:PHE:N	3:I:433:GLN:OE1	2.33	0.61
3:L:747:SER:OG	3:L:748:GLN:OE1	2.15	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:256:ASP:OD2	3:F:301:ASN:ND2	2.33	0.61
1:D:2:GLU:OE1	3:F:318:ARG:NH2	2.33	0.61
3:F:6:GLU:O	3:F:10:LEU:HB2	2.00	0.61
2:H:249:ARG:O	2:H:252:VAL:HG12	2.01	0.61
2:B:641:ASN:HA	2:B:652:ALA:HB1	1.83	0.61
1:D:208:THR:HG22	1:D:209:GLY:H	1.64	0.61
2:H:518:ASN:N	2:H:522:ASP:OD2	2.33	0.61
3:C:748:GLN:OE1	3:C:748:GLN:N	2.33	0.61
2:B:279:LYS:HA	2:B:282:LEU:HD12	1.82	0.61
2:B:89:LEU:HD21	2:B:320:ALA:HB1	1.82	0.61
2:B:77:HIS:CE1	2:B:479:LYS:HD2	2.36	0.61
3:C:141:ILE:HG21	3:C:143:ARG:HH21	1.66	0.61
1:G:483:ILE:HD12	1:G:504:ILE:HG22	1.83	0.61
3:I:488:TYR:CE2	3:I:490:SER:HB2	2.36	0.61
2:K:167:LEU:HD11	2:K:254:PHE:HE2	1.65	0.61
2:K:311:GLU:OE1	2:K:311:GLU:N	2.33	0.61
2:K:663:THR:O	2:K:666:TRP:NE1	2.34	0.61
1:A:54:ILE:HA	1:A:60:SER:HA	1.83	0.61
1:A:573:ILE:HA	1:A:576:LYS:HG2	1.83	0.61
1:D:302:ILE:HD12	1:D:303:PRO:HD2	1.82	0.61
2:H:307:THR:H	2:H:478:SER:HB2	1.66	0.61
2:K:564:GLY:HA2	2:K:577:LYS:HG2	1.83	0.61
1:A:78:ILE:HA	1:A:109:LEU:HD12	1.82	0.61
2:K:207:LYS:HB2	2:K:209:LYS:HG3	1.81	0.61
1:G:305:TYR:CZ	1:G:354:ILE:HG22	2.35	0.60
2:H:665:SER:HB2	3:I:47:MET:SD	2.40	0.60
3:I:610:PHE:HD2	3:I:615:ILE:HD11	1.64	0.60
1:J:48:TYR:CE1	1:J:163:LEU:HD11	2.35	0.60
3:L:504:VAL:HB	3:L:513:LEU:H	1.66	0.60
3:C:140:LYS:HB3	3:C:219:PRO:HB2	1.82	0.60
1:D:276:CYS:HA	1:D:401:ARG:HB3	1.83	0.60
1:D:594:SER:OG	2:E:16:ASN:O	2.16	0.60
1:J:343:ALA:O	1:J:347:ASP:N	2.34	0.60
2:E:752:GLU:O	2:E:756:GLN:NE2	2.34	0.60
2:H:429:LYS:HB3	2:H:437:TRP:HB3	1.83	0.60
3:I:664:ARG:HG2	3:I:674:ALA:HB2	1.84	0.60
1:A:217:GLN:NE2	2:B:59:THR:OG1	2.26	0.60
2:B:747:CYS:HA	2:B:750:ILE:HD12	1.83	0.60
2:E:63:ALA:HB1	2:E:402:SER:HB3	1.82	0.60
2:B:491:GLU:HG2	2:B:492:PHE:N	2.16	0.60
1:G:314:PHE:HD2	1:G:317:TRP:CE2	2.19	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:535:MET:HG2	3:I:536:MET:H	1.67	0.60
3:I:176:ILE:HD12	3:I:693:GLY:HA3	1.83	0.60
3:L:274:THR:O	3:L:500:ARG:NH1	2.34	0.60
2:E:297:GLU:OE2	2:E:437:TRP:NE1	2.33	0.60
1:J:618:THR:HB	1:J:630:GLU:HB3	1.84	0.60
2:K:669:LYS:O	3:L:46:ARG:NH1	2.33	0.60
1:D:31:GLU:OE1	1:D:200:THR:OG1	2.19	0.60
1:G:506:LYS:NZ	1:G:507:GLY:O	2.26	0.60
2:H:626:ASN:ND2	3:I:106:THR:OG1	2.35	0.60
2:K:174:MET:HA	2:K:217:TYR:HE2	1.67	0.60
2:K:427:GLY:HA3	2:K:438:TRP:CE2	2.36	0.60
2:E:491:GLU:HG2	2:E:492:PHE:N	2.17	0.60
1:G:251:LYS:O	1:G:254:ASN:ND2	2.33	0.60
1:G:477:MET:HG2	1:G:510:HIS:CD2	2.35	0.60
2:H:491:GLU:HG2	2:H:492:PHE:N	2.16	0.60
1:A:302:ILE:HD12	1:A:303:PRO:HD2	1.83	0.60
1:G:114:GLU:OE2	1:G:116:ARG:NH2	2.35	0.60
1:J:2:GLU:OE2	1:J:6:ARG:NH2	2.25	0.60
1:J:537:TRP:HB3	1:J:540:TYR:HB2	1.84	0.60
1:A:463:VAL:O	1:A:467:THR:OG1	2.10	0.60
2:B:52:LYS:O	2:B:54:LYS:NZ	2.32	0.60
3:F:140:LYS:HB3	3:F:219:PRO:HB2	1.82	0.60
1:G:573:ILE:HA	1:G:576:LYS:HG2	1.83	0.60
2:H:424:LEU:O	2:H:438:TRP:NE1	2.35	0.60
3:I:10:LEU:O	3:I:16:THR:OG1	2.14	0.60
3:I:748:GLN:N	3:I:748:GLN:OE1	2.35	0.60
2:K:269:SER:HB2	2:K:421:VAL:HG21	1.84	0.60
3:L:331:LYS:HE2	3:L:490:SER:H	1.67	0.60
2:B:663:THR:HB	2:B:666:TRP:HE1	1.67	0.59
2:E:50:SER:HB3	2:E:68:PRO:HG3	1.83	0.59
2:H:52:LYS:O	2:H:54:LYS:NZ	2.31	0.59
1:A:174:ARG:HE	1:A:178:ILE:HD11	1.67	0.59
1:G:208:THR:HG22	1:G:209:GLY:H	1.66	0.59
1:J:208:THR:HG22	1:J:209:GLY:H	1.67	0.59
1:J:318:LYS:NZ	1:J:544:GLU:OE2	2.35	0.59
1:A:672:LEU:HD23	1:A:678:PRO:HD2	1.85	0.59
3:F:614:GLN:NE2	3:F:649:VAL:O	2.28	0.59
3:I:141:ILE:HG21	3:I:143:ARG:HE	1.68	0.59
1:J:114:GLU:OE2	1:J:116:ARG:NH2	2.35	0.59
1:J:571:SER:H	1:J:574:LYS:HB2	1.67	0.59
2:K:307:THR:HA	2:K:481:LYS:HZ1	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:348:MET:HB3	2:B:400:THR:HB	1.84	0.59
3:C:71:ASN:OD1	3:C:75:GLN:N	2.30	0.59
2:E:70:ASP:OD2	2:E:85:THR:OG1	2.19	0.59
2:H:558:THR:HG23	3:I:48:LYS:HG2	1.85	0.59
2:H:623:ARG:NE	3:I:103:GLY:H	1.99	0.59
1:J:670:GLN:HG2	2:K:14:ALA:H	1.67	0.59
3:L:27:HIS:O	3:L:30:ILE:HG12	2.02	0.59
2:B:527:VAL:HA	2:B:530:ILE:HD12	1.83	0.59
3:C:27:HIS:O	3:C:30:ILE:HG12	2.02	0.59
3:C:665:LEU:HB3	3:C:672:ALA:O	2.02	0.59
2:E:307:THR:N	2:E:478:SER:HB2	2.17	0.59
2:H:563:ARG:HB2	2:H:580:TRP:HZ3	1.67	0.59
2:H:641:ASN:OD1	2:H:654:SER:OG	2.21	0.59
2:K:489:THR:HA	2:K:497:TYR:O	2.03	0.59
3:L:504:VAL:O	3:L:512:LEU:N	2.26	0.59
3:C:165:GLU:HG2	3:C:172:VAL:HG21	1.84	0.59
2:E:297:GLU:HA	2:E:454:PRO:HA	1.84	0.59
2:E:70:ASP:HB3	2:E:85:THR:H	1.68	0.59
3:F:754:ILE:HG13	3:F:755:ARG:HG2	1.85	0.59
2:H:438:TRP:HB2	2:H:449:LEU:HD11	1.85	0.59
2:B:579:LEU:HG	3:C:101:ARG:HB2	1.84	0.59
2:E:558:THR:HG23	3:F:48:LYS:HG2	1.83	0.59
2:K:252:VAL:HG23	2:K:412:PHE:CE1	2.37	0.59
1:J:213:ARG:NH2	2:K:60:GLU:OE2	2.35	0.59
1:A:504:ILE:HG12	1:A:522:SER:HA	1.84	0.59
2:E:310:ASN:O	2:E:310:ASN:ND2	2.36	0.59
2:E:410:GLY:H	2:E:413:ASN:HD21	1.49	0.59
3:I:581:GLN:OE1	3:I:589:ARG:NH1	2.36	0.59
1:J:321:ASN:ND2	1:J:544:GLU:OE1	2.35	0.59
2:B:309:TRP:HZ2	2:B:416:SER:HB3	1.68	0.59
2:B:519:GLU:HB3	2:B:664:HIS:CD2	2.38	0.59
1:G:154:GLU:OE2	1:G:168:ARG:HD2	2.03	0.59
3:I:505:ARG:NH1	3:I:509:GLY:O	2.35	0.59
2:K:303:THR:HG21	2:K:491:GLU:HB3	1.83	0.59
3:L:141:ILE:HG21	3:L:143:ARG:HH21	1.68	0.59
2:B:623:ARG:HD3	3:C:103:GLY:H	1.67	0.58
1:D:520:PHE:CE1	1:D:568:ASN:HB3	2.38	0.58
2:B:65:GLN:NE2	2:B:346:ASN:OD1	2.36	0.58
3:C:589:ARG:HG2	3:C:624:ALA:HB2	1.84	0.58
2:H:527:VAL:HA	2:H:530:ILE:HD12	1.84	0.58
3:L:138:GLN:O	3:L:140:LYS:NZ	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:292:ILE:HD11	1:A:310:CYS:SG	2.43	0.58
1:A:257:ILE:HD11	2:B:463:VAL:HG11	1.85	0.58
2:E:348:MET:HB3	2:E:400:THR:HB	1.83	0.58
2:E:575:GLU:OE2	3:F:101:ARG:NH1	2.36	0.58
1:J:324:LYS:HD2	1:J:325:PRO:HD2	1.85	0.58
1:J:587:GLN:HG2	1:J:591:GLN:NE2	2.19	0.58
2:H:708:PRO:CA	3:I:728:GLN:HE21	2.17	0.58
3:L:67:ILE:HG13	3:L:78:TRP:HZ2	1.66	0.58
1:D:398:PRO:HG2	1:D:695:ILE:HG21	1.86	0.58
3:F:446:PHE:HB3	3:F:465:PRO:HB3	1.85	0.58
3:F:664:ARG:NH2	3:F:671:ASP:OD2	2.35	0.58
3:I:274:THR:HG21	1:J:95:CYS:HB3	1.86	0.58
1:J:578:GLY:HA2	1:J:581:MET:HG3	1.85	0.58
1:D:321:ASN:ND2	1:D:544:GLU:OE1	2.36	0.58
1:G:618:THR:HB	1:G:630:GLU:HB3	1.83	0.58
1:J:111:ASP:OD1	1:J:114:GLU:N	2.35	0.58
1:J:261:LEU:O	1:J:265:PRO:HD3	2.04	0.58
2:K:549:GLN:HA	2:K:552:ILE:HD12	1.85	0.58
3:L:532:SER:OG	3:L:555:ARG:NH1	2.36	0.58
2:B:311:GLU:OE1	2:B:311:GLU:N	2.36	0.58
3:F:57:ILE:O	3:F:90:MET:HA	2.03	0.58
1:J:427:GLU:O	2:K:597:ASN:ND2	2.35	0.58
3:C:142:ARG:NH2	3:C:487:GLU:O	2.36	0.58
1:D:387:VAL:HB	1:D:390:LEU:HB2	1.85	0.58
2:H:428:GLN:HB2	2:H:430:ARG:HH21	1.68	0.58
3:I:610:PHE:CD2	3:I:615:ILE:HD11	2.38	0.58
1:J:612:PHE:HE1	1:J:633:ILE:HG21	1.68	0.58
2:K:710:GLY:N	3:L:26:ASP:OD1	2.34	0.58
1:A:462:GLY:O	1:A:466:ASN:ND2	2.34	0.58
2:E:527:VAL:HA	2:E:530:ILE:HD12	1.86	0.58
2:H:453:ALA:HB3	2:H:459:ILE:HG12	1.85	0.58
3:L:712:GLU:OE1	3:L:712:GLU:N	2.37	0.58
1:D:606:ASP:HB2	3:F:135:PHE:CG	2.39	0.58
1:D:612:PHE:CE1	1:D:633:ILE:HG21	2.39	0.58
2:E:602:ARG:HA	3:F:234:LEU:HD12	1.84	0.58
3:F:593:SER:HB2	3:F:624:ALA:HB3	1.84	0.58
2:K:374:ALA:HA	2:K:393:ARG:HE	1.68	0.58
2:B:389:ILE:HA	2:B:392:ILE:HG22	1.85	0.57
1:D:578:GLY:HA2	1:D:581:MET:HG3	1.86	0.57
1:D:587:GLN:HG2	1:D:591:GLN:NE2	2.19	0.57
3:L:365:MET:HE1	3:L:401:ALA:HB2	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:518:ASN:ND2	2:B:662:THR:O	2.36	0.57
1:J:262:LYS:O	1:J:716:ARG:NH1	2.31	0.57
1:J:530:PRO:HG3	1:J:542:VAL:HG21	1.86	0.57
1:J:94:ILE:O	1:J:98:THR:OG1	2.13	0.57
3:L:554:ILE:HD11	3:L:665:LEU:HD23	1.85	0.57
1:J:82:ARG:HH12	3:L:754:ILE:HA	1.69	0.57
2:H:316:ARG:NH2	2:H:345:SER:OG	2.37	0.57
3:L:557:TRP:HE3	3:L:616:ILE:HD11	1.68	0.57
1:A:1:MET:HA	1:A:187:LEU:HD13	1.86	0.57
2:B:623:ARG:NH1	3:C:101:ARG:O	2.37	0.57
2:K:222:LEU:HB3	2:K:347:LYS:HA	1.87	0.57
2:K:517:ILE:N	2:K:522:ASP:OD2	2.28	0.57
3:L:151:HIS:N	3:L:252:ASN:OD1	2.32	0.57
1:A:587:GLN:HG2	1:A:591:GLN:NE2	2.20	0.57
3:C:584:ILE:HD11	3:C:592:TYR:HD2	1.69	0.57
1:D:198:GLU:HG2	1:D:200:THR:HG22	1.86	0.57
1:G:612:PHE:CE1	1:G:633:ILE:HG21	2.40	0.57
1:A:483:ILE:HD12	1:A:504:ILE:HG22	1.86	0.57
3:C:362:GLU:HG3	3:C:375:ARG:HG2	1.87	0.57
2:E:326:THR:OG1	2:E:334:ARG:NE	2.29	0.57
2:H:708:PRO:CB	3:I:728:GLN:HE21	2.18	0.57
2:H:747:CYS:HA	2:H:750:ILE:HD12	1.86	0.57
1:J:116:ARG:NH1	1:J:162:THR:OG1	2.38	0.57
2:E:492:PHE:O	2:E:495:PHE:HB2	2.04	0.57
3:F:296:ASP:HA	3:F:299:ARG:HD2	1.86	0.57
2:H:563:ARG:HB2	2:H:580:TRP:CZ3	2.39	0.57
3:I:142:ARG:HB3	3:I:217:PHE:CE1	2.39	0.57
3:I:264:ARG:HH22	3:I:368:ARG:HH12	1.50	0.57
1:J:323:ILE:HG21	1:J:531:ARG:HH21	1.69	0.57
1:G:189:ASP:HA	2:H:162:ARG:NH1	2.20	0.57
3:I:264:ARG:NH1	3:I:520:GLU:HG2	2.20	0.57
3:I:371:THR:HG21	3:I:487:GLU:HG3	1.86	0.57
3:C:274:THR:HA	1:D:97:THR:HG23	1.87	0.57
1:J:173:THR:HG1	3:L:696:ILE:H	1.51	0.57
2:B:254:PHE:O	2:B:257:THR:OG1	2.21	0.57
2:B:727:ARG:O	2:B:731:GLU:HG3	2.05	0.57
2:E:289:MET:O	2:E:452:ASN:ND2	2.38	0.57
1:D:420:SER:HB2	1:D:422:TRP:CE2	2.40	0.56
1:J:31:GLU:OE1	1:J:200:THR:OG1	2.23	0.56
1:A:450:VAL:HG13	1:A:638:ARG:HG2	1.86	0.56
1:G:370:LEU:HD13	1:G:507:GLY:HA2	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:249:MET:HB3	2:K:468:ARG:HH21	1.70	0.56
2:B:434:THR:HG22	2:B:435:THR:H	1.70	0.56
3:C:426:GLN:NE2	1:D:96:ASN:O	2.38	0.56
2:E:509:LEU:HD23	2:E:509:LEU:H	1.70	0.56
3:F:366:VAL:HA	3:F:371:THR:HG22	1.87	0.56
1:G:596:ILE:O	1:G:600:SER:OG	2.15	0.56
2:K:374:ALA:O	2:K:393:ARG:NH2	2.37	0.56
2:B:572:ARG:NH2	3:C:97:THR:OG1	2.37	0.56
3:C:736:LYS:HE2	3:C:738:LYS:HG2	1.88	0.56
1:D:647:ASN:OD1	1:D:699:TRP:NE1	2.23	0.56
2:E:114:VAL:HG12	2:E:254:PHE:CE1	2.40	0.56
2:E:640:ALA:HB3	2:E:654:SER:HB3	1.87	0.56
2:E:70:ASP:HA	2:E:84:GLN:HA	1.87	0.56
2:K:287:ARG:O	2:K:291:THR:OG1	2.17	0.56
3:C:19:ILE:HD11	3:C:31:ILE:HD11	1.88	0.56
1:D:491:THR:OG1	1:D:495:ARG:N	2.36	0.56
2:E:727:ARG:O	2:E:731:GLU:HG3	2.06	0.56
3:F:335:GLY:HA3	3:F:361:GLU:HA	1.87	0.56
1:G:528:THR:O	1:G:564:TYR:OH	2.16	0.56
2:H:303:THR:HG21	2:H:491:GLU:HB3	1.86	0.56
2:H:666:TRP:HB2	3:I:58:THR:HG22	1.88	0.56
1:J:455:ALA:HB1	1:J:645:VAL:HG21	1.86	0.56
3:L:700:GLU:HB2	3:L:731:VAL:HB	1.87	0.56
1:A:288:LEU:HG	1:A:527:LEU:HG	1.88	0.56
3:F:725:LEU:HA	3:F:731:VAL:HA	1.87	0.56
2:H:664:HIS:HA	3:I:57:ILE:HG13	1.87	0.56
2:H:572:ARG:NH2	3:I:97:THR:OG1	2.32	0.56
2:B:606:ILE:HD13	3:C:122:VAL:HG22	1.88	0.56
3:C:496:VAL:HA	3:C:506:ASP:HA	1.87	0.56
2:E:77:HIS:CE1	2:E:479:LYS:HD2	2.41	0.56
1:A:58:GLY:N	3:F:628:GLN:H	2.03	0.56
1:J:261:LEU:O	1:J:264:THR:OG1	2.19	0.56
2:K:491:GLU:HG2	2:K:492:PHE:N	2.21	0.56
3:L:360:TYR:OH	3:L:375:ARG:NE	2.38	0.56
3:L:329:THR:HG23	3:L:366:VAL:HB	1.87	0.56
2:B:249:ARG:O	2:B:252:VAL:HG12	2.06	0.56
2:B:114:VAL:HG12	2:B:254:PHE:CE1	2.41	0.56
2:B:517:ILE:N	2:B:522:ASP:OD2	2.34	0.56
1:D:108:ASP:HB2	1:D:119:GLU:HA	1.86	0.56
1:D:427:GLU:OE2	2:E:556:ARG:NH1	2.32	0.56
1:D:431:ASP:OD1	2:E:600:ASN:ND2	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:387:SER:HB3	3:F:485:VAL:HG23	1.87	0.56
1:G:483:ILE:HD11	1:G:506:LYS:HB2	1.88	0.56
2:H:527:VAL:HG11	2:H:599:TYR:HD2	1.71	0.56
2:K:294:GLN:O	2:K:296:THR:N	2.37	0.56
3:L:301:ASN:OD1	3:L:303:THR:OG1	2.18	0.56
1:A:215:ALA:HB1	1:A:226:LEU:HD13	1.88	0.56
1:D:292:ILE:HD11	1:D:310:CYS:SG	2.46	0.56
3:F:237:GLY:HA3	3:F:240:TRP:CE2	2.40	0.56
1:J:584:CYS:O	1:J:588:SER:OG	2.20	0.56
3:C:361:GLU:OE1	3:C:376:LYS:NZ	2.29	0.56
3:C:409:CYS:SG	3:C:449:TRP:HA	2.46	0.56
1:D:447:THR:O	1:D:451:SER:N	2.38	0.56
2:E:554:ASP:O	2:E:558:THR:OG1	2.13	0.56
3:F:301:ASN:OD1	3:F:303:THR:OG1	2.15	0.56
3:F:606:VAL:O	3:F:609:THR:OG1	2.23	0.56
1:G:124:ARG:NH1	1:G:194:SER:OG	2.39	0.56
1:G:36:ALA:O	1:G:40:THR:OG1	2.23	0.56
1:J:130:TYR:HB3	1:J:147:ILE:HD13	1.88	0.56
1:J:78:ILE:HA	1:J:109:LEU:CD1	2.35	0.56
3:F:264:ARG:HH12	3:F:520:GLU:HG2	1.70	0.56
1:G:288:LEU:HD12	1:G:289:LYS:H	1.71	0.56
1:G:293:GLU:HA	1:G:497:LYS:HA	1.88	0.56
1:G:52:HIS:CD2	1:G:163:LEU:HD21	2.40	0.56
1:J:520:PHE:CE1	1:J:568:ASN:HB3	2.41	0.56
2:K:132:THR:HG21	2:K:145:ASN:HB3	1.87	0.56
2:K:219:ILE:HG23	2:K:348:MET:HG3	1.87	0.56
3:L:374:LEU:HD11	3:L:381:LEU:HG	1.88	0.56
2:H:315:PRO:HA	2:H:318:PHE:HD2	1.70	0.55
1:J:262:LYS:HB2	1:J:716:ARG:HB2	1.88	0.55
2:K:453:ALA:HB3	2:K:459:ILE:HG12	1.87	0.55
2:K:554:ASP:O	2:K:558:THR:OG1	2.11	0.55
2:K:589:LEU:HA	2:K:620:TYR:CE2	2.40	0.55
1:A:338:TRP:HE1	1:A:545:ILE:HD11	1.70	0.55
1:A:522:SER:O	1:A:565:VAL:HA	2.05	0.55
2:B:252:VAL:HG23	2:B:412:PHE:HE1	1.71	0.55
3:C:497:SER:OG	3:C:505:ARG:O	2.23	0.55
3:F:71:ASN:OD1	3:F:75:GLN:N	2.30	0.55
1:G:54:ILE:HD13	1:G:113:LYS:HG2	1.89	0.55
3:I:385:ILE:HA	3:I:479:ARG:HB2	1.88	0.55
3:L:534:SER:OG	3:L:535:MET:SD	2.61	0.55
1:G:89:THR:HG21	3:L:755:ARG:HH12	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:573:ILE:HA	1:D:576:LYS:HG2	1.87	0.55
1:J:189:ASP:HA	2:K:162:ARG:NH1	2.17	0.55
3:L:141:ILE:O	3:L:219:PRO:HA	2.06	0.55
2:H:518:ASN:O	2:H:559:TYR:OH	2.21	0.55
2:K:612:LYS:O	2:K:616:MET:HG3	2.07	0.55
2:B:248:ILE:HG21	2:B:344:PHE:CE1	2.41	0.55
1:D:427:GLU:O	2:E:597:ASN:ND2	2.31	0.55
2:E:658:ASP:OD1	2:E:659:ALA:N	2.40	0.55
3:I:744:LEU:HD12	3:I:746:ASP:H	1.71	0.55
2:K:225:ASN:O	2:K:243:THR:N	2.40	0.55
2:K:316:ARG:NH2	2:K:345:SER:OG	2.40	0.55
1:A:589:LEU:O	1:A:593:GLU:N	2.33	0.55
1:D:483:ILE:HD11	1:D:506:LYS:HB2	1.88	0.55
1:D:658:PHE:HD1	1:D:694:LEU:HD11	1.71	0.55
1:G:530:PRO:HB3	1:G:564:TYR:HE1	1.72	0.55
2:H:289:MET:O	2:H:452:ASN:ND2	2.39	0.55
1:J:602:VAL:O	1:J:603:LYS:HE2	2.07	0.55
3:F:428:LEU:HB2	3:F:433:GLN:HE21	1.70	0.55
3:F:721:LYS:HE2	3:F:733:LEU:HD22	1.88	0.55
1:G:111:ASP:OD1	1:G:114:GLU:N	2.39	0.55
1:J:166:GLU:OE2	1:J:170:ARG:NH1	2.29	0.55
1:G:302:ILE:HD12	1:G:303:PRO:HD2	1.87	0.55
3:I:27:HIS:O	3:I:30:ILE:HG12	2.07	0.55
3:I:593:SER:HB2	3:I:624:ALA:HB3	1.89	0.55
2:K:438:TRP:HB2	2:K:449:LEU:HD11	1.88	0.55
2:B:419:LEU:O	2:B:422:SER:OG	2.19	0.55
2:B:670:ARG:HD3	2:B:670:ARG:H	1.72	0.55
3:C:747:SER:OG	3:C:748:GLN:OE1	2.19	0.55
2:E:690:GLN:OE1	3:F:35:THR:OG1	2.23	0.55
3:F:142:ARG:HB3	3:F:217:PHE:CZ	2.42	0.55
2:H:151:ARG:HE	3:I:18:GLU:CD	2.09	0.55
2:H:583:THR:O	2:H:586:LYS:NZ	2.24	0.55
3:L:335:GLY:HA3	3:L:361:GLU:HA	1.88	0.55
3:L:352:LEU:HD22	3:L:430:PRO:HG3	1.88	0.55
1:A:307:ALA:HA	1:A:310:CYS:SG	2.47	0.55
2:E:572:ARG:HA	3:F:94:LEU:HD12	1.88	0.55
2:H:136:ASN:OD1	2:H:225:ASN:ND2	2.40	0.55
3:I:57:ILE:O	3:I:90:MET:HA	2.06	0.55
1:J:549:LEU:H	1:J:549:LEU:HD23	1.72	0.55
1:J:672:LEU:HD23	1:J:678:PRO:HD2	1.89	0.55
3:C:436:ARG:NH1	3:C:439:GLN:OE1	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:531:LYS:NZ	2:E:532:ASN:OD1	2.31	0.54
1:G:449:GLU:O	1:G:638:ARG:NH2	2.40	0.54
1:G:549:LEU:HD23	1:G:549:LEU:H	1.72	0.54
3:I:408:ASP:O	3:I:412:LYS:HG2	2.07	0.54
3:I:142:ARG:NH1	3:I:488:TYR:HB2	2.22	0.54
1:J:323:ILE:HD11	1:J:544:GLU:HB2	1.89	0.54
2:K:336:VAL:HG12	2:K:337:LEU:HD23	1.89	0.54
2:K:434:THR:HG22	2:K:435:THR:H	1.72	0.54
2:B:181:ILE:HD11	2:B:212:LEU:HD22	1.90	0.54
2:B:252:VAL:HG23	2:B:412:PHE:CE1	2.43	0.54
3:C:446:PHE:CB	3:C:465:PRO:HB3	2.37	0.54
1:D:164:ASP:OD1	1:D:165:GLU:N	2.34	0.54
3:F:559:THR:O	3:F:562:ILE:HD12	2.07	0.54
3:L:593:SER:HB2	3:L:624:ALA:HB3	1.90	0.54
3:I:559:THR:O	3:I:563:GLN:HB2	2.08	0.54
3:L:332:ARG:HA	3:L:363:PHE:CD1	2.42	0.54
3:L:542:PRO:HB2	3:L:640:VAL:HG12	1.89	0.54
1:A:344:GLU:OE1	1:A:358:LYS:NZ	2.28	0.54
2:E:98:SER:OG	2:E:431:TYR:OH	2.25	0.54
2:H:54:LYS:HG3	2:H:68:PRO:HA	1.87	0.54
2:K:120:ASP:OD1	3:L:30:ILE:HA	2.08	0.54
2:E:68:PRO:HD2	2:E:314:ASN:HD21	1.73	0.54
3:F:664:ARG:HG2	3:F:674:ALA:HB2	1.89	0.54
3:F:703:ARG:NH2	3:F:704:TYR:OH	2.37	0.54
2:H:691:LYS:NZ	3:I:6:GLU:OE2	2.32	0.54
1:J:54:ILE:HD13	1:J:113:LYS:HG2	1.90	0.54
1:J:573:ILE:HA	1:J:576:LYS:HG2	1.89	0.54
1:J:84:ARG:HE	1:J:88:TRP:HD1	1.53	0.54
2:K:589:LEU:HA	2:K:620:TYR:HE2	1.73	0.54
3:C:327:GLY:HA2	3:C:368:ARG:HH21	1.73	0.54
3:F:70:ARG:HG3	3:F:74:GLY:HA2	1.90	0.54
2:H:430:ARG:HD3	3:I:360:TYR:HB3	1.89	0.54
2:K:304:GLY:HA2	2:K:482:SER:HA	1.89	0.54
3:L:101:ARG:NE	3:L:102:ASN:OD1	2.21	0.54
2:K:691:LYS:NZ	3:L:6:GLU:OE2	2.37	0.54
1:A:164:ASP:OD1	1:A:165:GLU:N	2.39	0.54
1:A:240:GLY:N	2:B:90:GLU:OE1	2.32	0.54
1:D:261:LEU:O	1:D:264:THR:OG1	2.25	0.54
2:B:671:ASN:HD22	3:C:38:ARG:HH12	1.54	0.54
2:E:279:LYS:HA	2:E:282:LEU:HD12	1.89	0.54
3:F:371:THR:OG1	3:F:487:GLU:OE2	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:535:MET:O	3:C:537:TRP:N	2.41	0.54
1:D:111:ASP:OD1	1:D:114:GLU:N	2.40	0.54
2:E:323:THR:O	2:E:334:ARG:NH2	2.37	0.54
3:I:301:ASN:OD1	3:I:303:THR:OG1	2.16	0.54
2:H:697:GLU:OE2	3:I:32:LYS:NZ	2.41	0.54
1:J:189:ASP:O	1:J:193:GLN:NE2	2.38	0.54
3:L:461:ILE:HD12	3:L:469:PRO:HB3	1.88	0.54
1:A:635:LYS:O	1:A:639:THR:OG1	2.15	0.53
2:E:103:PHE:HB3	2:E:325:ILE:HG23	1.90	0.53
2:H:65:GLN:NE2	2:H:345:SER:O	2.41	0.53
3:I:71:ASN:OD1	3:I:75:GLN:N	2.27	0.53
1:J:387:VAL:HB	1:J:390:LEU:HB2	1.90	0.53
2:K:509:LEU:HD23	2:K:509:LEU:H	1.72	0.53
3:F:374:LEU:HD11	3:F:381:LEU:HG	1.90	0.53
1:G:134:LYS:HB3	1:G:145:ILE:HD13	1.90	0.53
1:J:274:PRO:O	1:J:402:SER:N	2.33	0.53
3:L:283:MET:O	3:L:287:THR:N	2.39	0.53
3:L:748:GLN:N	3:L:748:GLN:OE1	2.40	0.53
1:A:606:ASP:HB2	3:C:135:PHE:CG	2.42	0.53
2:B:305:ASP:HB2	2:B:446:ASP:OD1	2.09	0.53
2:B:90:GLU:HG2	2:B:94:PHE:CZ	2.42	0.53
3:C:331:LYS:HE2	3:C:490:SER:H	1.73	0.53
3:I:115:TYR:CE1	3:I:206:MET:HG3	2.43	0.53
1:A:469:LEU:HG	1:A:483:ILE:HD13	1.89	0.53
2:B:638:GLU:HG2	2:B:656:GLU:HG2	1.90	0.53
1:D:196:ARG:HG3	1:D:201:ILE:HD13	1.90	0.53
2:E:59:THR:OG1	2:E:60:GLU:OE1	2.19	0.53
1:G:592:ILE:O	1:G:596:ILE:HG13	2.09	0.53
2:H:527:VAL:HG11	2:H:599:TYR:CD2	2.43	0.53
1:A:527:LEU:HB3	1:A:559:ARG:HH22	1.73	0.53
1:G:310:CYS:O	1:G:313:THR:OG1	2.25	0.53
1:G:26:GLU:HG3	1:G:31:GLU:HG3	1.89	0.53
1:G:420:SER:HB3	1:G:489:CYS:HB2	1.90	0.53
3:I:586:LYS:HG2	3:I:589:ARG:NH2	2.23	0.53
3:L:629:SER:OG	3:L:631:MET:SD	2.54	0.53
1:A:353:LYS:HB3	1:G:353:LYS:HB3	1.89	0.53
1:A:549:LEU:H	1:A:549:LEU:HD23	1.72	0.53
2:E:269:SER:HB2	2:E:421:VAL:HG21	1.89	0.53
3:F:151:HIS:HB2	3:F:211:LEU:O	2.09	0.53
2:K:271:LEU:HD11	2:K:443:SER:HA	1.90	0.53
2:K:575:GLU:OE2	3:L:101:ARG:NH1	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:71:ASN:OD1	3:L:75:GLN:N	2.28	0.53
2:B:663:THR:O	2:B:666:TRP:NE1	2.42	0.53
3:C:540:ASN:OD1	3:C:541:GLY:N	2.40	0.53
3:C:57:ILE:HB	3:C:91:VAL:O	2.08	0.53
1:D:110:TYR:HB2	1:D:117:PHE:CE1	2.44	0.53
1:D:36:ALA:O	1:D:40:THR:OG1	2.24	0.53
2:E:428:GLN:HE21	2:E:431:TYR:HE1	1.57	0.53
3:F:264:ARG:HH22	3:F:368:ARG:HH12	1.56	0.53
3:F:562:ILE:HD12	3:F:563:GLN:H	1.73	0.53
1:G:215:ALA:HB1	1:G:226:LEU:HD23	1.90	0.53
3:L:366:VAL:HA	3:L:371:THR:HG22	1.90	0.53
1:A:442:ARG:HE	1:A:596:ILE:HG21	1.74	0.53
1:A:715:LEU:C	1:A:716:ARG:HE	2.11	0.53
2:E:287:ARG:O	2:E:291:THR:OG1	2.19	0.53
2:E:605:HIS:HD2	3:F:233:HIS:NE2	2.06	0.53
2:H:746:ILE:O	2:H:750:ILE:HG13	2.09	0.53
3:I:449:TRP:NE1	3:I:476:ARG:HB3	2.22	0.53
1:J:54:ILE:HA	1:J:60:SER:HA	1.89	0.53
2:K:578:LYS:HE3	3:L:101:ARG:NH1	2.24	0.53
3:L:535:MET:SD	3:L:535:MET:N	2.82	0.53
2:K:578:LYS:NZ	3:L:72:GLU:OE2	2.32	0.53
2:B:630:PRO:HB2	3:C:60:ASP:OD1	2.08	0.53
1:D:606:ASP:HB2	3:F:135:PHE:CD1	2.43	0.53
3:F:276:PRO:HD2	3:F:500:ARG:NH2	2.23	0.53
2:H:727:ARG:O	2:H:731:GLU:HG3	2.09	0.53
1:G:7:GLN:NE2	3:I:296:ASP:OD1	2.35	0.53
2:K:96:GLU:OE1	2:K:324:TYR:OH	2.14	0.53
3:L:135:PHE:CE2	3:L:240:TRP:HB3	2.44	0.53
1:A:283:LEU:O	1:A:461:LYS:NZ	2.38	0.53
1:A:520:PHE:CE1	1:A:568:ASN:HB3	2.44	0.53
2:B:307:THR:H	2:B:478:SER:HB2	1.74	0.53
3:C:746:ASP:O	3:C:749:THR:OG1	2.25	0.53
1:D:547:ASP:HA	1:D:560:PRO:HA	1.90	0.53
1:G:283:LEU:HG	1:G:524:GLU:HG2	1.91	0.53
3:I:115:TYR:HD1	3:I:118:TYR:HE2	1.56	0.53
2:K:153:ASN:HB2	2:K:155:LEU:HD12	1.91	0.53
3:L:659:ASN:HB2	3:L:662:THR:HB	1.90	0.53
3:C:231:VAL:HG11	3:C:244:TYR:HE2	1.74	0.52
1:G:46:PHE:CD2	3:I:750:ALA:HB1	2.44	0.52
2:B:420:GLY:HA3	2:B:442:GLN:HG2	1.91	0.52
2:B:704:SER:O	3:C:205:TYR:OH	2.22	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:268:GLN:NE2	2:E:439:ASP:OD1	2.43	0.52
2:E:65:GLN:HB3	2:E:404:SER:HB2	1.91	0.52
1:G:274:PRO:O	1:G:402:SER:N	2.40	0.52
1:G:500:LEU:HD21	1:G:503:PHE:HE1	1.74	0.52
1:D:504:ILE:HG12	1:D:522:SER:HA	1.91	0.52
2:E:579:LEU:HA	2:E:582:GLN:HG2	1.92	0.52
1:G:537:TRP:HB3	1:G:540:TYR:HB2	1.91	0.52
2:K:668:PRO:HB2	3:L:46:ARG:HH11	1.74	0.52
2:E:65:GLN:NE2	2:E:346:ASN:OD1	2.42	0.52
1:G:53:PHE:HB3	1:G:71:LEU:HD22	1.91	0.52
2:H:514:VAL:HG11	2:H:558:THR:HG21	1.91	0.52
1:J:48:TYR:CD1	1:J:163:LEU:HD11	2.44	0.52
3:L:142:ARG:HB2	3:L:487:GLU:O	2.09	0.52
3:L:429:ASN:OD1	3:L:432:HIS:ND1	2.42	0.52
1:D:624:SER:OG	1:D:625:PRO:HD3	2.10	0.52
2:E:397:ILE:O	2:E:400:THR:OG1	2.26	0.52
2:H:531:LYS:HD2	3:I:233:HIS:ND1	2.25	0.52
2:H:589:LEU:HA	2:H:620:TYR:HE2	1.74	0.52
1:J:362:LYS:HG3	1:J:480:PHE:HE1	1.75	0.52
3:C:750:ALA:O	3:C:754:ILE:HG22	2.09	0.52
1:G:151:THR:HG22	2:H:711:ILE:HD13	1.92	0.52
1:G:520:PHE:CE1	1:G:568:ASN:HB3	2.45	0.52
1:G:587:GLN:HG2	1:G:591:GLN:NE2	2.24	0.52
2:H:110:THR:O	2:H:114:VAL:HG13	2.09	0.52
2:H:99:HIS:NE2	3:I:333:THR:O	2.42	0.52
3:F:652:ASN:OD1	3:F:658:TYR:N	2.36	0.52
2:K:658:ASP:OD1	2:K:659:ALA:N	2.42	0.52
2:B:305:ASP:OD1	2:B:306:ASN:N	2.34	0.52
1:D:483:ILE:HD12	1:D:504:ILE:HG22	1.90	0.52
2:E:96:GLU:OE1	2:E:324:TYR:OH	2.17	0.52
1:D:576:LYS:NZ	3:F:42:ASN:OD1	2.42	0.52
2:K:589:LEU:HD23	2:K:620:TYR:CZ	2.45	0.52
1:A:58:GLY:HA3	3:F:627:GLU:HA	1.91	0.52
2:B:449:LEU:HD22	2:B:466:PHE:CD2	2.45	0.52
2:B:600:ASN:OD1	2:B:601:ILE:N	2.38	0.52
3:C:387:SER:OG	3:C:485:VAL:N	2.43	0.52
3:C:586:LYS:HG2	3:C:589:ARG:NH2	2.23	0.52
2:H:114:VAL:HG12	2:H:254:PHE:CD1	2.44	0.52
3:I:332:ARG:HA	3:I:363:PHE:CD1	2.45	0.52
3:C:237:GLY:HA3	3:C:240:TRP:CE2	2.45	0.52
2:E:518:ASN:OD1	2:E:520:SER:N	2.38	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:605:HIS:CE1	2:H:606:ILE:HG13	2.45	0.52
1:G:11:PRO:HG2	3:I:285:HIS:NE2	2.24	0.52
2:K:306:ASN:HA	2:K:478:SER:H	1.74	0.52
3:L:360:TYR:HE1	3:L:375:ARG:HB3	1.74	0.52
1:D:491:THR:HG22	1:D:497:LYS:HE3	1.90	0.51
3:F:257:GLN:NE2	3:F:524:THR:O	2.43	0.51
1:G:302:ILE:HG12	1:G:305:TYR:CD2	2.45	0.51
2:H:389:ILE:HA	2:H:392:ILE:HG22	1.91	0.51
1:A:125:ARG:HD3	1:A:195:GLU:HG3	1.91	0.51
3:C:627:GLU:O	3:C:629:SER:N	2.43	0.51
3:F:141:ILE:HG13	3:F:487:GLU:OE1	2.10	0.51
1:J:249:MET:HB2	2:K:73:LEU:HD13	1.92	0.51
1:A:592:ILE:O	1:A:596:ILE:HG13	2.11	0.51
1:A:681:PHE:HB2	2:B:479:LYS:O	2.11	0.51
2:E:382:ASN:ND2	2:E:385:THR:OG1	2.44	0.51
1:J:36:ALA:O	1:J:40:THR:OG1	2.24	0.51
1:J:276:CYS:HA	1:J:401:ARG:HB3	1.92	0.51
1:J:444:ASN:OD1	1:J:445:TYR:N	2.42	0.51
3:L:338:VAL:HB	3:L:358:GLU:HB3	1.92	0.51
3:L:563:GLN:HG2	3:L:571:LEU:HB2	1.92	0.51
2:B:708:PRO:HB3	3:C:728:GLN:HG3	1.92	0.51
2:B:711:ILE:O	3:C:24:THR:OG1	2.26	0.51
3:C:655:VAL:HG22	3:C:668:LEU:HD21	1.93	0.51
2:E:88:VAL:HG11	2:E:317:MET:HG3	1.93	0.51
2:E:579:LEU:HG	3:F:101:ARG:HB2	1.91	0.51
3:F:138:GLN:O	3:F:140:LYS:NZ	2.43	0.51
3:F:708:LEU:O	3:F:724:VAL:HG23	2.10	0.51
1:G:362:LYS:HG3	1:G:480:PHE:CE1	2.45	0.51
3:I:144:ARG:HG3	3:I:489:SER:HB2	1.93	0.51
3:I:135:PHE:CZ	3:I:240:TRP:HB3	2.44	0.51
3:I:379:ARG:NH1	3:I:408:ASP:OD2	2.44	0.51
1:J:658:PHE:CD1	1:J:694:LEU:HD11	2.44	0.51
1:A:571:SER:H	1:A:574:LYS:HB2	1.76	0.51
2:B:158:ASN:N	2:B:169:ASP:OD2	2.43	0.51
2:B:212:LEU:HD21	2:B:217:TYR:HD1	1.75	0.51
2:B:449:LEU:HD22	2:B:466:PHE:HD2	1.75	0.51
1:G:324:LYS:NZ	1:G:540:TYR:O	2.41	0.51
3:I:429:ASN:OD1	3:I:432:HIS:ND1	2.43	0.51
1:J:370:LEU:HD13	1:J:507:GLY:HA2	1.90	0.51
3:L:454:ILE:HD13	3:L:474:SER:HB3	1.93	0.51
3:L:463:ILE:HD11	3:L:467:MET:HA	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:331:ASN:N	1:A:332:PRO:HD2	2.25	0.51
3:C:337:SER:OG	3:C:361:GLU:OE2	2.25	0.51
3:F:147:VAL:N	3:F:214:LYS:O	2.44	0.51
3:F:568:PRO:HB2	3:F:572:TYR:CZ	2.45	0.51
2:H:326:THR:HB	2:H:334:ARG:HG2	1.93	0.51
3:L:163:ILE:O	3:L:167:VAL:HG12	2.11	0.51
3:L:408:ASP:O	3:L:412:LYS:HG2	2.10	0.51
3:L:617:LYS:NZ	3:L:648:LEU:O	2.37	0.51
1:J:169:ALA:HB1	3:L:696:ILE:O	2.10	0.51
2:B:336:VAL:HG12	2:B:337:LEU:HD23	1.92	0.51
3:C:412:LYS:O	3:C:415:ARG:NH1	2.28	0.51
1:D:52:HIS:O	1:D:75:ARG:HB3	2.10	0.51
2:E:319:LEU:HB2	2:E:341:PRO:HB2	1.92	0.51
2:E:632:VAL:HA	2:E:663:THR:HG21	1.92	0.51
2:E:291:THR:O	3:F:383:GLN:NE2	2.44	0.51
1:G:305:TYR:HH	1:G:356:LYS:H	1.57	0.51
1:J:324:LYS:NZ	1:J:327:GLU:HG3	2.25	0.51
1:J:670:GLN:OE1	1:J:673:ARG:NH2	2.42	0.51
2:K:600:ASN:OD1	2:K:601:ILE:N	2.38	0.51
3:L:584:ILE:HD11	3:L:592:TYR:HD2	1.75	0.51
3:F:301:ASN:O	3:F:312:LYS:NZ	2.43	0.51
1:G:198:GLU:HG2	1:G:200:THR:HG22	1.92	0.51
3:I:138:GLN:O	3:I:140:LYS:NZ	2.44	0.51
1:J:420:SER:HB2	1:J:422:TRP:CE2	2.46	0.51
1:J:95:CYS:O	1:J:99:GLY:N	2.44	0.51
2:B:658:ASP:OD1	2:B:659:ALA:N	2.43	0.51
2:B:602:ARG:HA	3:C:234:LEU:HD12	1.93	0.51
2:B:576:LEU:HD12	3:C:97:THR:HG21	1.92	0.51
2:E:605:HIS:CE1	2:E:606:ILE:HG13	2.45	0.51
2:K:626:ASN:HD21	2:K:628:LEU:HB2	1.75	0.51
3:L:142:ARG:HB3	3:L:217:PHE:CE1	2.45	0.51
3:I:655:VAL:O	3:I:667:VAL:HA	2.11	0.51
2:K:77:HIS:CE1	2:K:479:LYS:HD2	2.46	0.51
1:A:314:PHE:HB3	1:A:317:TRP:CZ2	2.46	0.50
3:C:420:PHE:O	3:C:433:GLN:NE2	2.44	0.50
2:E:58:ASN:OD1	2:E:61:THR:N	2.31	0.50
2:E:689:TYR:HD1	3:F:31:ILE:HD11	1.75	0.50
3:F:414:VAL:O	3:F:415:ARG:NH1	2.33	0.50
2:H:254:PHE:O	2:H:257:THR:OG1	2.23	0.50
2:H:517:ILE:N	2:H:522:ASP:OD2	2.34	0.50
3:I:261:ILE:HD13	3:I:524:THR:N	2.25	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:139:LYS:HG2	1:A:140:SER:H	1.76	0.50
2:E:310:ASN:OD1	2:E:409:MET:N	2.44	0.50
3:F:55:TYR:CE1	3:F:77:LEU:HA	2.43	0.50
1:D:169:ALA:HB1	3:F:696:ILE:O	2.11	0.50
1:G:73:LYS:HE3	1:G:112:TYR:CE2	2.46	0.50
1:G:620:PRO:HD2	2:H:11:LYS:HB2	1.93	0.50
2:H:50:SER:HB3	2:H:68:PRO:HG3	1.93	0.50
2:K:305:ASP:N	2:K:481:LYS:O	2.45	0.50
2:K:710:GLY:O	3:L:26:ASP:N	2.43	0.50
3:L:296:ASP:OD1	3:L:299:ARG:NH1	2.44	0.50
3:L:584:ILE:HD11	3:L:592:TYR:CD2	2.46	0.50
3:L:646:ARG:HH22	3:L:648:LEU:HD21	1.76	0.50
1:A:469:LEU:O	1:A:473:SER:OG	2.24	0.50
1:A:74:HIS:C	1:A:76:PHE:H	2.13	0.50
2:B:605:HIS:HD2	3:C:233:HIS:NE2	2.09	0.50
2:B:605:HIS:CE1	2:B:606:ILE:HG13	2.46	0.50
2:B:751:GLU:OE2	2:B:755:ARG:NH2	2.44	0.50
3:C:265:ASN:OD1	3:C:268:ARG:NH1	2.44	0.50
3:F:704:TYR:CB	3:F:721:LYS:HZ1	2.20	0.50
2:H:52:LYS:HB3	2:H:54:LYS:HZ3	1.77	0.50
1:J:624:SER:OG	1:J:625:PRO:HD3	2.12	0.50
2:K:90:GLU:HG2	2:K:94:PHE:CE2	2.46	0.50
1:A:714:ALA:O	1:A:716:ARG:HG2	2.12	0.50
2:B:318:PHE:HA	2:B:321:MET:HG2	1.92	0.50
2:B:457:GLU:OE1	2:B:457:GLU:N	2.44	0.50
1:D:219:LEU:O	2:E:316:ARG:NH1	2.43	0.50
1:G:590:GLN:HB3	2:H:543:THR:HG21	1.92	0.50
2:H:52:LYS:HB3	2:H:54:LYS:NZ	2.27	0.50
2:H:600:ASN:OD1	2:H:601:ILE:N	2.40	0.50
3:I:142:ARG:HB2	3:I:487:GLU:O	2.12	0.50
1:J:483:ILE:HD12	1:J:504:ILE:HG22	1.92	0.50
3:L:357:HIS:ND1	3:L:406:GLN:OE1	2.39	0.50
2:B:514:VAL:HG22	2:B:516:GLY:H	1.77	0.50
1:D:314:PHE:HD2	1:D:317:TRP:CE2	2.28	0.50
2:E:278:LYS:HD2	2:E:495:PHE:CZ	2.46	0.50
2:E:434:THR:CG2	2:E:435:THR:H	2.17	0.50
2:H:100:PRO:HB3	3:I:508:ARG:NH1	2.26	0.50
2:H:305:ASP:OD1	2:H:306:ASN:N	2.38	0.50
2:H:449:LEU:HD22	2:H:466:PHE:HD2	1.76	0.50
1:J:75:ARG:HG3	1:J:76:PHE:CD2	2.47	0.50
2:K:59:THR:OG1	2:K:60:GLU:OE1	2.30	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:584:ILE:HG13	3:L:585:PRO:HD2	1.93	0.50
3:L:694:PHE:HD1	3:L:736:LYS:HA	1.75	0.50
3:L:736:LYS:HG3	3:L:738:LYS:HZ3	1.76	0.50
3:L:79:SER:OG	3:L:80:LYS:N	2.45	0.50
2:E:326:THR:HB	2:E:329:GLN:HB2	1.93	0.50
1:G:169:ALA:HA	1:G:172:LYS:HE3	1.94	0.50
1:G:522:SER:O	1:G:565:VAL:HA	2.11	0.50
1:G:266:ARG:HG3	1:G:687:TYR:CE2	2.46	0.50
1:J:265:PRO:HD2	1:J:716:ARG:NH1	2.26	0.50
3:L:282:GLU:O	3:L:286:SER:HB3	2.12	0.50
1:D:549:LEU:HD23	1:D:549:LEU:H	1.75	0.50
1:G:624:SER:OG	1:G:625:PRO:HD3	2.12	0.50
2:H:620:TYR:O	2:H:624:LEU:HB2	2.12	0.50
2:K:110:THR:HG21	2:K:337:LEU:HD11	1.93	0.50
2:K:518:ASN:OD1	2:K:520:SER:N	2.41	0.50
1:A:274:PRO:O	1:A:402:SER:N	2.45	0.50
2:B:153:ASN:HB2	2:B:155:LEU:HD12	1.93	0.50
2:B:339:ILE:O	2:B:343:MET:HG3	2.12	0.50
1:A:179:ARG:NH1	2:B:711:ILE:HG13	2.26	0.50
3:C:550:TYR:O	3:C:554:ILE:HG13	2.12	0.50
1:D:443:ARG:HG3	1:D:444:ASN:N	2.27	0.50
1:D:479:ASP:N	1:D:479:ASP:OD1	2.45	0.50
1:D:54:ILE:HG13	1:D:75:ARG:HB2	1.94	0.50
2:E:434:THR:HG21	2:E:436:TYR:CE2	2.47	0.50
2:H:531:LYS:NZ	2:H:532:ASN:OD1	2.34	0.50
2:K:67:ASN:HD21	2:K:316:ARG:NH1	2.09	0.50
3:L:744:LEU:HD12	3:L:746:ASP:H	1.77	0.50
1:A:261:LEU:O	1:A:265:PRO:HD3	2.12	0.50
1:A:426:ASP:OD1	2:B:553:LYS:HB2	2.12	0.50
2:B:712:SER:OG	3:C:730:ASP:HB3	2.12	0.50
1:D:431:ASP:OD2	1:D:440:SER:HB2	2.12	0.50
1:D:528:THR:O	1:D:564:TYR:OH	2.14	0.50
2:E:15:GLN:OE1	2:E:498:ARG:NH2	2.38	0.50
3:F:272:VAL:HG22	3:F:424:ALA:HB2	1.94	0.50
1:G:621:ILE:HG21	1:G:636:VAL:HG22	1.94	0.50
1:J:169:ALA:HA	1:J:172:LYS:HE3	1.92	0.50
1:J:513:ASN:HB2	1:J:516:ASP:OD1	2.11	0.50
3:L:655:VAL:O	3:L:667:VAL:HA	2.11	0.50
2:B:110:THR:O	2:B:114:VAL:HG13	2.12	0.49
2:B:78:GLU:O	2:B:471:LYS:NZ	2.45	0.49
1:D:331:ASN:N	1:D:332:PRO:HD2	2.26	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:146:ASP:HA	3:F:215:THR:HA	1.94	0.49
1:G:184:SER:OG	2:H:706:ARG:NH2	2.45	0.49
1:G:180:GLN:NE2	3:I:174:ALA:H	2.10	0.49
1:J:446:PHE:CE1	1:J:637:CYS:HB3	2.47	0.49
3:C:235:THR:O	3:C:241:GLU:HA	2.12	0.49
3:C:55:TYR:CD1	3:C:92:SER:HB2	2.46	0.49
3:F:16:THR:HA	3:F:19:ILE:HG22	1.94	0.49
3:F:141:ILE:O	3:F:219:PRO:HA	2.12	0.49
1:G:523:MET:HB3	1:G:563:LEU:HD11	1.94	0.49
2:K:534:MET:HE1	2:K:601:ILE:HG12	1.94	0.49
1:J:426:ASP:OD1	2:K:553:LYS:HB2	2.12	0.49
1:A:114:GLU:OE2	1:A:116:ARG:NH2	2.45	0.49
1:A:7:GLN:OE1	1:A:185:ARG:NH2	2.46	0.49
2:B:57:THR:HA	2:B:64:PRO:HA	1.95	0.49
3:C:331:LYS:HE2	3:C:490:SER:N	2.28	0.49
1:D:135:ALA:O	1:D:139:LYS:HB2	2.13	0.49
1:D:326:HIS:ND1	1:D:326:HIS:O	2.44	0.49
2:E:142:ALA:O	2:E:146:THR:OG1	2.24	0.49
2:E:711:ILE:O	3:F:24:THR:OG1	2.28	0.49
1:G:205:PHE:HE2	2:H:339:ILE:HD11	1.76	0.49
1:J:196:ARG:HG3	1:J:201:ILE:HD13	1.95	0.49
2:K:77:HIS:NE2	2:K:479:LYS:HD2	2.27	0.49
2:K:727:ARG:O	2:K:731:GLU:HG3	2.12	0.49
3:L:193:LEU:HA	3:L:196:CYS:SG	2.52	0.49
3:L:364:THR:HG22	3:L:373:ILE:HD12	1.94	0.49
3:L:449:TRP:NE1	3:L:476:ARG:HB3	2.27	0.49
3:F:610:PHE:HD2	3:F:615:ILE:HD11	1.76	0.49
3:F:542:PRO:HB2	3:F:640:VAL:HG12	1.93	0.49
2:H:519:GLU:O	2:H:555:TYR:OH	2.19	0.49
2:H:658:ASP:OD1	2:H:659:ALA:N	2.45	0.49
2:K:151:ARG:HH21	3:L:18:GLU:HG3	1.77	0.49
3:L:57:ILE:O	3:L:90:MET:HA	2.13	0.49
1:A:444:ASN:OD1	1:A:445:TYR:N	2.45	0.49
1:A:523:MET:HG2	1:A:565:VAL:HG22	1.95	0.49
2:B:443:SER:OG	2:B:444:SER:N	2.45	0.49
1:D:302:ILE:HG23	1:D:305:TYR:HB2	1.93	0.49
3:F:577:PHE:O	3:F:581:GLN:N	2.41	0.49
2:H:397:ILE:O	2:H:400:THR:OG1	2.27	0.49
3:I:443:LYS:O	3:I:447:GLN:HG2	2.13	0.49
3:I:535:MET:HG2	3:I:536:MET:N	2.27	0.49
1:J:523:MET:HG2	1:J:565:VAL:HG22	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:318:LYS:HB2	1:J:546:GLY:HA2	1.94	0.49
1:A:213:ARG:NH2	2:B:60:GLU:OE2	2.46	0.49
1:A:76:PHE:HA	1:A:110:TYR:O	2.12	0.49
3:C:430:PRO:O	3:C:434:LEU:HG	2.13	0.49
2:E:89:LEU:HD21	2:E:320:ALA:HB1	1.95	0.49
3:F:111:TYR:O	3:F:113:LYS:N	2.39	0.49
2:K:114:VAL:HG12	2:K:254:PHE:CD1	2.47	0.49
1:A:111:ASP:OD1	1:A:114:GLU:N	2.46	0.49
1:A:624:SER:OG	1:A:625:PRO:HD3	2.13	0.49
2:B:693:CYS:SG	3:C:31:ILE:HG23	2.52	0.49
1:D:444:ASN:OD1	1:D:445:TYR:N	2.45	0.49
2:E:347:LYS:HZ1	2:E:406:GLY:H	1.60	0.49
2:H:492:PHE:O	2:H:495:PHE:HB2	2.12	0.49
2:H:509:LEU:H	2:H:509:LEU:HD23	1.77	0.49
2:H:706:ARG:NH1	3:I:161:ASP:OD1	2.44	0.49
1:J:457:GLU:OE2	1:J:501:TYR:OH	2.23	0.49
1:J:479:ASP:OD1	1:J:479:ASP:N	2.43	0.49
2:K:224:LEU:N	2:K:348:MET:O	2.45	0.49
2:K:583:THR:O	2:K:586:LYS:NZ	2.34	0.49
3:L:325:PHE:CZ	3:L:431:MET:HB3	2.47	0.49
1:A:120:ILE:HA	1:A:146:HIS:O	2.13	0.49
2:B:589:LEU:HA	2:B:620:TYR:CE2	2.48	0.49
2:B:716:GLU:HA	2:B:754:ARG:HH12	1.78	0.49
2:E:110:THR:O	2:E:114:VAL:HG13	2.11	0.49
2:E:315:PRO:HA	2:E:318:PHE:HD2	1.78	0.49
2:E:443:SER:OG	2:E:444:SER:N	2.45	0.49
1:G:611:PHE:HE1	1:G:619:TRP:CZ2	2.30	0.49
1:G:427:GLU:OE2	2:H:556:ARG:NH1	2.46	0.49
3:I:77:LEU:O	3:I:78:TRP:HD1	1.95	0.49
2:K:696:PHE:CE2	2:K:703:SER:HB3	2.48	0.49
2:B:307:THR:N	2:B:478:SER:HB2	2.28	0.49
3:C:535:MET:HG2	3:C:536:MET:N	2.27	0.49
2:E:470:CYS:HB3	2:E:475:ILE:O	2.13	0.49
1:G:418:THR:HG21	1:G:454:ARG:HD3	1.95	0.49
2:H:523:MET:HA	2:H:551:PHE:HZ	1.78	0.49
3:I:159:ALA:O	3:I:163:ILE:HG12	2.13	0.49
1:J:621:ILE:HD11	1:J:631:GLY:HA3	1.95	0.49
2:K:289:MET:C	2:K:452:ASN:HD21	2.16	0.49
2:K:371:GLU:OE1	2:K:371:GLU:N	2.45	0.49
3:L:384:LEU:HB3	3:L:478:VAL:HA	1.95	0.49
3:C:135:PHE:CZ	3:C:240:TRP:HB3	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:474:CYS:HB2	3:C:49:TRP:CH2	2.48	0.49
3:F:27:HIS:O	3:F:30:ILE:HG12	2.13	0.49
3:F:446:PHE:HB3	3:F:465:PRO:CB	2.42	0.49
2:H:410:GLY:H	2:H:413:ASN:HD21	1.59	0.49
3:I:327:GLY:N	3:I:517:GLU:OE1	2.35	0.49
1:J:307:ALA:HA	1:J:310:CYS:SG	2.53	0.49
1:J:257:ILE:HD13	2:K:460:GLN:HG3	1.95	0.49
2:K:70:ASP:N	2:K:83:ALA:O	2.33	0.49
3:L:636:LEU:HB2	3:L:647:ILE:HG23	1.95	0.49
1:G:331:ASN:N	1:G:332:PRO:HD2	2.28	0.48
2:H:77:HIS:CE1	2:H:479:LYS:HD2	2.48	0.48
2:H:589:LEU:HD23	2:H:620:TYR:CE2	2.48	0.48
3:I:142:ARG:HB3	3:I:217:PHE:CZ	2.47	0.48
1:J:606:ASP:HB2	3:L:135:PHE:CG	2.48	0.48
2:B:623:ARG:CD	3:C:103:GLY:H	2.26	0.48
2:H:225:ASN:ND2	2:H:350:ARG:HD3	2.28	0.48
3:I:593:SER:O	3:I:597:ARG:HG3	2.14	0.48
1:J:427:GLU:OE2	2:K:556:ARG:NH1	2.44	0.48
3:L:170:ASN:OD1	3:L:709:SER:OG	2.26	0.48
3:L:412:LYS:O	3:L:415:ARG:NH1	2.32	0.48
3:L:694:PHE:CD1	3:L:736:LYS:HA	2.48	0.48
1:D:149:PRO:HG3	1:D:153:GLU:HB2	1.94	0.48
2:E:514:VAL:HG22	2:E:516:GLY:H	1.77	0.48
1:G:294:ASP:N	1:G:294:ASP:OD1	2.47	0.48
1:G:420:SER:HB2	1:G:422:TRP:CE2	2.48	0.48
1:G:444:ASN:OD1	1:G:445:TYR:N	2.46	0.48
3:I:36:SER:HB3	3:I:38:ARG:HG3	1.96	0.48
2:K:572:ARG:HA	3:L:94:LEU:HD21	1.95	0.48
2:K:690:GLN:OE1	3:L:35:THR:OG1	2.19	0.48
3:L:753:ARG:HD2	3:L:753:ARG:HA	1.58	0.48
2:B:111:MET:HA	2:B:114:VAL:HG22	1.95	0.48
2:B:224:LEU:N	2:B:348:MET:O	2.46	0.48
2:B:531:LYS:HA	2:B:534:MET:HE3	1.96	0.48
2:B:578:LYS:HG2	3:C:101:ARG:HH11	1.77	0.48
3:C:635:SER:HB2	3:C:646:ARG:HH11	1.79	0.48
2:H:125:GLY:HA3	2:H:249:ARG:HH22	1.79	0.48
2:H:88:VAL:HG22	2:H:473:VAL:HG12	1.94	0.48
3:I:275:ASP:HB3	1:J:96:ASN:ND2	2.23	0.48
2:K:305:ASP:OD1	2:K:306:ASN:N	2.37	0.48
2:K:518:ASN:N	2:K:522:ASP:OD2	2.39	0.48
3:L:354:ILE:HD12	3:L:430:PRO:HB2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:77:LEU:O	3:L:78:TRP:HD1	1.96	0.48
3:C:268:ARG:HG2	3:C:423:ARG:HH12	1.78	0.48
1:D:297:HIS:HA	1:D:496:ARG:HH11	1.76	0.48
2:E:746:ILE:O	2:E:750:ILE:HG13	2.13	0.48
3:F:260:ILE:O	3:F:264:ARG:HG3	2.13	0.48
1:G:54:ILE:HD11	1:G:75:ARG:HD3	1.96	0.48
3:I:227:VAL:O	3:I:231:VAL:HG22	2.13	0.48
3:I:606:VAL:O	3:I:609:THR:OG1	2.31	0.48
3:I:70:ARG:HG3	3:I:74:GLY:HA2	1.96	0.48
1:J:618:THR:HB	1:J:630:GLU:CB	2.43	0.48
1:A:472:ALA:O	1:A:476:ALA:N	2.36	0.48
3:C:377:ALA:HB3	3:C:380:ARG:HB2	1.95	0.48
3:C:454:ILE:HD13	3:C:474:SER:HB3	1.95	0.48
2:E:303:THR:HG21	2:E:491:GLU:HB3	1.95	0.48
1:G:82:ARG:HG2	3:I:754:ILE:HD13	1.95	0.48
1:G:667:LEU:HD11	2:H:496:PHE:HE2	1.79	0.48
3:I:352:LEU:HD22	3:I:430:PRO:HG3	1.96	0.48
1:J:622:GLY:HA2	2:K:3:VAL:HA	1.94	0.48
2:K:248:ILE:HD13	2:K:344:PHE:HE1	1.78	0.48
1:A:366:LEU:HD21	1:A:505:ILE:HD13	1.96	0.48
1:A:95:CYS:O	1:A:99:GLY:N	2.47	0.48
1:D:10:ASN:HD21	1:D:13:ILE:HG13	1.79	0.48
1:J:366:LEU:HD21	1:J:505:ILE:HD13	1.94	0.48
1:J:522:SER:O	1:J:565:VAL:HA	2.14	0.48
2:K:160:SER:OG	2:K:165:ASP:OD2	2.29	0.48
1:A:31:GLU:HB3	1:A:34:LYS:HB3	1.95	0.48
1:A:457:GLU:OE2	1:A:501:TYR:OH	2.20	0.48
2:E:371:GLU:N	2:E:371:GLU:OE1	2.47	0.48
1:G:52:HIS:NE2	1:G:163:LEU:HD11	2.29	0.48
1:G:96:ASN:OD1	3:L:274:THR:OG1	2.31	0.48
3:I:344:VAL:HG11	3:I:411:ILE:HD12	1.94	0.48
1:J:305:TYR:CZ	1:J:354:ILE:HG22	2.49	0.48
1:J:440:SER:HA	1:J:443:ARG:HG2	1.94	0.48
2:K:371:GLU:HG3	2:K:399:GLY:HA3	1.96	0.48
3:L:296:ASP:HA	3:L:299:ARG:HD2	1.94	0.48
1:A:209:GLY:C	1:A:211:MET:H	2.17	0.48
1:A:491:THR:OG1	1:A:495:ARG:N	2.47	0.48
1:D:130:TYR:CE1	1:D:197:GLY:HA2	2.48	0.48
1:D:205:PHE:CD1	2:E:168:LYS:HG2	2.49	0.48
2:E:252:VAL:HG23	2:E:412:PHE:CE1	2.48	0.48
3:F:344:VAL:HB	3:F:352:LEU:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:292:ILE:HD11	1:G:310:CYS:SG	2.53	0.48
3:I:124:ARG:HH12	3:I:149:PRO:HG3	1.77	0.48
2:K:65:GLN:HB3	2:K:404:SER:HB2	1.96	0.48
1:D:369:ALA:HB1	1:D:521:VAL:HG21	1.95	0.48
2:E:600:ASN:OD1	2:E:601:ILE:N	2.40	0.48
3:F:323:PHE:HB3	3:F:330:PHE:HB2	1.96	0.48
1:G:307:ALA:HA	1:G:310:CYS:SG	2.53	0.48
1:J:124:ARG:NH2	1:J:190:SER:OG	2.47	0.48
3:L:115:TYR:CE1	3:L:206:MET:HG3	2.48	0.48
1:A:621:ILE:HD11	1:A:631:GLY:HA3	1.95	0.47
1:A:82:ARG:NH2	3:C:753:ARG:O	2.39	0.47
2:H:443:SER:OG	2:H:444:SER:N	2.46	0.47
3:L:140:LYS:HB3	3:L:219:PRO:HB2	1.95	0.47
1:A:273:GLY:N	1:A:402:SER:HB3	2.28	0.47
1:A:73:LYS:HE3	1:A:112:TYR:CE2	2.49	0.47
2:B:182:THR:HG22	2:B:209:LYS:HG2	1.94	0.47
3:C:142:ARG:HH22	3:C:488:TYR:HD1	1.60	0.47
1:D:276:CYS:HB2	1:D:698:PRO:HG3	1.96	0.47
2:E:163:LEU:O	2:E:167:LEU:HG	2.14	0.47
3:F:695:LEU:O	3:F:734:VAL:HA	2.14	0.47
2:H:77:HIS:O	2:H:77:HIS:ND1	2.44	0.47
3:I:354:ILE:HD11	3:I:431:MET:HG2	1.96	0.47
3:I:360:TYR:OH	3:I:375:ARG:NE	2.47	0.47
3:I:430:PRO:O	3:I:434:LEU:HG	2.14	0.47
1:D:445:TYR:HD2	1:D:612:PHE:CD2	2.32	0.47
1:G:73:LYS:HD2	1:G:73:LYS:HA	1.62	0.47
1:G:86:MET:O	1:G:90:VAL:HG23	2.15	0.47
2:H:225:ASN:OD1	2:H:226:THR:N	2.39	0.47
1:J:385:LYS:HG3	1:J:386:ASP:OD1	2.14	0.47
2:K:77:HIS:ND1	2:K:77:HIS:O	2.46	0.47
1:A:583:ARG:HH11	2:B:25:THR:HG21	1.80	0.47
2:B:212:LEU:HD21	2:B:217:TYR:CD1	2.49	0.47
2:B:95:LEU:HA	2:B:425:ASN:ND2	2.28	0.47
2:E:368:ILE:O	2:E:368:ILE:HD12	2.14	0.47
1:D:667:LEU:HD13	2:E:483:TYR:OH	2.15	0.47
2:H:96:GLU:OE1	2:H:324:TYR:OH	2.21	0.47
1:J:362:LYS:HG3	1:J:480:PHE:CE1	2.49	0.47
2:K:256:GLU:OE1	2:K:414:MET:HB2	2.14	0.47
2:K:565:ASP:HB2	2:K:580:TRP:CH2	2.48	0.47
3:L:172:VAL:HG12	3:L:710:ILE:HD13	1.96	0.47
3:L:55:TYR:HA	3:L:91:VAL:C	2.34	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:412:PHE:O	2:B:416:SER:OG	2.28	0.47
2:B:746:ILE:O	2:B:750:ILE:HG13	2.14	0.47
3:C:225:SER:O	3:C:229:ILE:HG12	2.13	0.47
3:C:257:GLN:NE2	3:C:526:ARG:HB3	2.28	0.47
3:C:652:ASN:OD1	3:C:658:TYR:N	2.35	0.47
1:D:624:SER:HB3	2:E:2:ASP:H	1.80	0.47
2:E:629:ASN:OD1	2:E:632:VAL:N	2.40	0.47
2:E:700:PHE:O	2:E:703:SER:OG	2.30	0.47
1:G:188:TRP:CD1	1:G:191:PHE:HB2	2.49	0.47
3:I:664:ARG:NH2	3:I:671:ASP:OD2	2.47	0.47
2:K:427:GLY:HA3	2:K:438:TRP:NE1	2.30	0.47
2:K:520:SER:HB3	2:K:662:THR:HG21	1.96	0.47
3:L:430:PRO:O	3:L:434:LEU:HG	2.14	0.47
1:A:455:ALA:O	1:A:459:ILE:HG13	2.15	0.47
1:A:287:ALA:HA	1:A:525:PHE:O	2.14	0.47
3:C:700:GLU:HB2	3:C:731:VAL:HB	1.95	0.47
2:E:449:LEU:HG	2:E:450:ILE:N	2.28	0.47
3:F:547:VAL:HG12	3:F:667:VAL:HG23	1.95	0.47
2:H:625:CYS:HB3	3:I:111:TYR:CZ	2.49	0.47
1:J:528:THR:O	1:J:564:TYR:OH	2.24	0.47
1:J:707:PHE:O	1:J:711:LEU:HG	2.14	0.47
2:K:457:GLU:OE1	2:K:457:GLU:N	2.47	0.47
2:K:574:PHE:HZ	2:K:578:LYS:HZ1	1.62	0.47
2:B:518:ASN:N	2:B:522:ASP:OD2	2.39	0.47
2:B:686:GLU:O	2:B:686:GLU:HG2	2.15	0.47
2:B:120:ASP:OD2	3:C:30:ILE:HA	2.15	0.47
1:G:512:ARG:N	1:G:516:ASP:OD2	2.48	0.47
1:G:276:CYS:HB2	1:G:698:PRO:HG3	1.97	0.47
2:H:612:LYS:O	2:H:616:MET:HG3	2.14	0.47
3:I:482:LYS:HE2	3:I:483:MET:HE1	1.97	0.47
2:K:464:ASP:O	2:K:468:ARG:HG2	2.13	0.47
2:K:58:ASN:OD1	2:K:61:THR:N	2.35	0.47
2:K:578:LYS:HE3	3:L:101:ARG:HH12	1.79	0.47
2:K:623:ARG:HD3	3:L:103:GLY:H	1.80	0.47
3:L:135:PHE:CZ	3:L:240:TRP:HB3	2.50	0.47
3:L:261:ILE:HD13	3:L:524:THR:H	1.78	0.47
3:L:293:ARG:HE	3:L:743:ILE:HG21	1.79	0.47
1:A:75:ARG:HG3	1:A:76:PHE:CD2	2.50	0.47
2:B:449:LEU:HG	2:B:450:ILE:N	2.29	0.47
1:A:583:ARG:NH1	2:B:509:LEU:O	2.46	0.47
1:D:366:LEU:HD12	1:D:366:LEU:HA	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:323:ILE:HD11	1:D:544:GLU:HB2	1.95	0.47
1:D:73:LYS:HD2	1:D:73:LYS:HA	1.62	0.47
2:E:516:GLY:N	2:E:522:ASP:OD1	2.47	0.47
3:F:225:SER:OG	3:F:226:SER:N	2.48	0.47
1:G:95:CYS:O	1:G:99:GLY:N	2.48	0.47
3:I:111:TYR:O	3:I:113:LYS:N	2.44	0.47
2:B:225:ASN:O	2:B:243:THR:N	2.48	0.47
2:B:273:VAL:O	2:B:278:LYS:NZ	2.40	0.47
2:B:716:GLU:HG3	2:B:754:ARG:HH22	1.79	0.47
1:D:139:LYS:HG2	1:D:140:SER:H	1.80	0.47
1:D:587:GLN:NE2	2:E:25:THR:OG1	2.48	0.47
2:E:419:LEU:O	2:E:422:SER:OG	2.16	0.47
2:E:531:LYS:O	2:E:535:ILE:HG12	2.14	0.47
2:H:432:THR:HA	2:H:465:ARG:NH1	2.30	0.47
3:I:410:MET:HE1	3:I:434:LEU:HD13	1.97	0.47
1:J:331:ASN:N	1:J:332:PRO:HD2	2.29	0.47
2:K:129:TYR:OH	2:K:134:ASN:OD1	2.15	0.47
1:A:234:ASP:O	2:B:327:ARG:NH2	2.48	0.47
2:B:330:PRO:O	2:B:334:ARG:HG3	2.15	0.47
2:B:623:ARG:HD3	3:C:103:GLY:N	2.30	0.47
3:C:429:ASN:OD1	3:C:432:HIS:ND1	2.48	0.47
3:C:584:ILE:HG13	3:C:585:PRO:HD2	1.96	0.47
2:E:629:ASN:HB2	2:E:631:PHE:CD2	2.49	0.47
1:G:297:HIS:HA	1:G:496:ARG:HH12	1.79	0.47
1:J:435:ILE:O	1:J:438:ILE:N	2.48	0.47
3:L:721:LYS:HA	3:L:734:VAL:O	2.15	0.47
3:C:752:LYS:HA	3:C:752:LYS:HD3	1.66	0.47
2:E:653:LYS:NZ	3:F:216:ARG:HH12	2.13	0.47
3:F:557:TRP:CZ3	3:F:616:ILE:HD11	2.50	0.47
1:G:28:PRO:HB3	1:G:35:PHE:HD2	1.80	0.47
1:G:446:PHE:O	1:G:450:VAL:HG23	2.14	0.47
1:G:54:ILE:O	1:G:71:LEU:HD21	2.14	0.47
3:I:747:SER:O	3:I:750:ALA:HB3	2.14	0.47
2:K:712:SER:OG	3:L:730:ASP:HB3	2.15	0.47
3:C:124:ARG:HB3	3:C:246:PRO:HB3	1.97	0.46
3:C:225:SER:OG	3:C:226:SER:N	2.48	0.46
2:E:310:ASN:ND2	2:E:407:MET:O	2.48	0.46
3:F:744:LEU:HD12	3:F:746:ASP:H	1.79	0.46
1:G:587:GLN:O	1:G:591:GLN:NE2	2.36	0.46
1:G:660:ALA:HA	1:G:663:ARG:NH1	2.29	0.46
2:H:90:GLU:HG2	2:H:94:PHE:CE2	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:523:MET:HB3	1:J:563:LEU:HD11	1.96	0.46
2:K:666:TRP:CG	3:L:58:THR:HG22	2.50	0.46
2:B:112:GLU:O	2:B:116:GLN:NE2	2.48	0.46
3:C:327:GLY:N	3:C:517:GLU:OE1	2.34	0.46
1:D:595:MET:HG2	2:E:17:ALA:HB2	1.97	0.46
1:G:249:MET:SD	2:H:468:ARG:NE	2.89	0.46
2:H:419:LEU:O	2:H:422:SER:OG	2.22	0.46
2:H:657:TYR:OH	3:I:209:ARG:NH2	2.49	0.46
2:K:309:TRP:CH2	2:K:416:SER:HB3	2.51	0.46
2:K:319:LEU:O	2:K:323:THR:OG1	2.27	0.46
2:K:514:VAL:HG22	2:K:516:GLY:H	1.79	0.46
1:A:266:ARG:O	1:A:687:TYR:OH	2.20	0.46
1:A:305:TYR:OH	1:A:354:ILE:HG22	2.15	0.46
2:B:397:ILE:O	2:B:400:THR:OG1	2.29	0.46
2:B:285:VAL:HG21	2:B:441:LEU:HD11	1.97	0.46
3:C:617:LYS:HD2	3:C:656:PHE:CD2	2.50	0.46
2:E:339:ILE:O	2:E:343:MET:HG3	2.15	0.46
3:F:165:GLU:HG2	3:F:172:VAL:HG21	1.96	0.46
1:G:597:GLU:O	1:G:601:SER:N	2.48	0.46
2:K:305:ASP:OD1	2:K:445:ASP:HB2	2.16	0.46
3:L:269:ARG:HH21	3:L:535:MET:HG3	1.80	0.46
1:A:527:LEU:HB3	1:A:559:ARG:NH2	2.31	0.46
2:B:591:VAL:N	2:B:608:GLU:OE2	2.41	0.46
2:E:102:ILE:HD11	2:E:265:LYS:HB2	1.96	0.46
2:E:219:ILE:HG23	2:E:348:MET:HG3	1.97	0.46
3:I:154:LEU:HD11	3:I:185:ILE:HD12	1.97	0.46
2:K:174:MET:HA	2:K:217:TYR:CE2	2.47	0.46
2:K:273:VAL:O	2:K:278:LYS:NZ	2.44	0.46
3:L:110:HIS:NE2	3:L:196:CYS:HB2	2.30	0.46
1:A:354:ILE:HA	1:A:355:PRO:HD3	1.74	0.46
2:B:374:ALA:C	2:B:393:ARG:HH21	2.18	0.46
3:C:38:ARG:HD3	3:C:39:GLN:N	2.30	0.46
1:D:454:ARG:HG2	1:D:458:TYR:CZ	2.50	0.46
1:D:522:SER:O	1:D:565:VAL:HA	2.16	0.46
2:E:305:ASP:OD1	2:E:306:ASN:N	2.40	0.46
2:E:527:VAL:HG11	2:E:599:TYR:CE2	2.50	0.46
2:H:204:THR:OG1	2:H:205:ILE:N	2.49	0.46
3:I:193:LEU:HA	3:I:196:CYS:SG	2.56	0.46
3:I:599:LEU:HA	3:I:599:LEU:HD23	1.81	0.46
2:K:316:ARG:HG2	2:K:316:ARG:H	1.59	0.46
2:K:449:LEU:HD13	2:K:466:PHE:CE2	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:543:GLU:CD	3:L:641:ARG:HE	2.19	0.46
1:A:292:ILE:HG22	1:A:294:ASP:HB2	1.97	0.46
3:C:128:GLY:HA3	3:C:244:TYR:HE1	1.81	0.46
1:D:326:HIS:C	1:D:328:LYS:H	2.18	0.46
1:D:351:GLU:OE1	1:D:358:LYS:NZ	2.38	0.46
2:E:54:LYS:HG3	2:E:68:PRO:HA	1.97	0.46
2:E:90:GLU:HG2	2:E:94:PHE:CE2	2.50	0.46
1:G:209:GLY:C	1:G:211:MET:H	2.19	0.46
2:H:449:LEU:HG	2:H:450:ILE:N	2.29	0.46
1:J:74:HIS:C	1:J:76:PHE:H	2.19	0.46
1:A:118:ILE:HG12	1:A:144:HIS:HB3	1.97	0.46
2:B:310:ASN:OD1	2:B:409:MET:N	2.49	0.46
3:C:581:GLN:OE1	3:C:589:ARG:NH1	2.49	0.46
3:C:77:LEU:HD12	3:C:78:TRP:CD1	2.51	0.46
3:C:79:SER:OG	3:C:80:LYS:N	2.49	0.46
2:K:270:GLY:O	2:K:278:LYS:NZ	2.46	0.46
3:L:237:GLY:HA3	3:L:240:TRP:CE2	2.51	0.46
1:A:449:GLU:OE1	1:A:634:GLY:HA3	2.16	0.46
3:C:80:LYS:HE3	3:C:80:LYS:HB2	1.84	0.46
1:D:380:ASP:HB2	1:D:382:GLU:HG2	1.98	0.46
1:D:179:ARG:NH1	2:E:711:ILE:HG13	2.31	0.46
3:F:67:ILE:HG22	3:F:98:TRP:CZ3	2.51	0.46
2:H:336:VAL:HG12	2:H:337:LEU:HD23	1.98	0.46
3:I:31:ILE:HG13	3:I:34:TYR:CE2	2.51	0.46
2:K:249:ARG:HA	2:K:252:VAL:HG12	1.98	0.46
2:K:663:THR:HB	2:K:666:TRP:CZ2	2.50	0.46
1:A:366:LEU:HA	1:A:366:LEU:HD12	1.63	0.46
2:B:534:MET:HE2	2:B:534:MET:HB2	1.66	0.46
2:E:589:LEU:HD23	2:E:620:TYR:CE2	2.50	0.46
2:E:572:ARG:NH2	3:F:97:THR:OG1	2.49	0.46
1:G:135:ALA:O	1:G:139:LYS:HB2	2.16	0.46
1:G:584:CYS:O	1:G:588:SER:OG	2.27	0.46
1:G:670:GLN:NE2	1:G:674:ASP:OD1	2.49	0.46
2:H:427:GLY:HA3	2:H:438:TRP:CE2	2.51	0.46
3:L:115:TYR:HB3	3:L:118:TYR:HD2	1.81	0.46
2:B:24:TYR:CE2	2:B:28:PRO:HG3	2.51	0.46
2:B:334:ARG:O	2:B:338:SER:OG	2.21	0.46
3:C:141:ILE:O	3:C:219:PRO:HA	2.16	0.46
1:D:324:LYS:NZ	1:D:325:PRO:O	2.30	0.46
3:F:305:GLU:O	3:F:309:ASP:N	2.31	0.46
3:F:721:LYS:CE	3:F:733:LEU:HD22	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:326:HIS:C	1:G:328:LYS:H	2.18	0.46
2:H:449:LEU:HD22	2:H:466:PHE:CD2	2.51	0.46
3:I:151:HIS:HB2	3:I:211:LEU:O	2.15	0.46
3:I:267:VAL:O	3:I:271:THR:HG23	2.16	0.46
3:L:292:ILE:HB	3:L:297:ILE:HD11	1.98	0.46
1:A:670:GLN:OE1	1:A:673:ARG:NH2	2.46	0.45
3:C:54:LYS:HG2	3:C:54:LYS:H	1.54	0.45
3:C:557:TRP:CE3	3:C:616:ILE:HD11	2.51	0.45
1:D:676:LEU:HB3	2:E:486:ARG:HB2	1.98	0.45
2:E:94:PHE:HB3	2:E:431:TYR:CE2	2.50	0.45
3:I:402:MET:HE3	3:I:402:MET:HB2	1.75	0.45
1:J:181:GLU:OE2	3:L:157:LYS:HD2	2.15	0.45
2:K:225:ASN:OD1	2:K:226:THR:N	2.39	0.45
3:L:745:THR:HA	3:L:748:GLN:HB2	1.97	0.45
1:A:124:ARG:NH1	1:A:194:SER:OG	2.50	0.45
1:A:506:LYS:NZ	1:A:507:GLY:O	2.25	0.45
2:B:523:MET:HA	2:B:551:PHE:HZ	1.82	0.45
2:E:519:GLU:HB3	2:E:664:HIS:CE1	2.51	0.45
2:E:708:PRO:HD2	3:F:28:ILE:HG22	1.97	0.45
3:F:128:GLY:HA2	3:F:246:PRO:HA	1.97	0.45
3:F:264:ARG:NH2	3:F:368:ARG:HH12	2.13	0.45
3:F:28:ILE:O	3:F:31:ILE:HG22	2.16	0.45
1:G:283:LEU:O	1:G:461:LYS:NZ	2.44	0.45
1:G:681:PHE:HB3	2:H:479:LYS:HE2	1.99	0.45
2:H:708:PRO:HB3	3:I:728:GLN:NE2	2.29	0.45
3:I:429:ASN:OD1	3:I:429:ASN:N	2.49	0.45
3:I:57:ILE:HB	3:I:91:VAL:O	2.16	0.45
1:J:418:THR:HG21	1:J:454:ARG:HD3	1.96	0.45
1:A:303:PRO:O	1:A:486:ILE:HD11	2.17	0.45
2:B:129:TYR:HE2	2:B:350:ARG:HD3	1.81	0.45
2:B:322:ILE:HD12	2:B:341:PRO:HG2	1.97	0.45
3:C:301:ASN:OD1	3:C:303:THR:OG1	2.18	0.45
3:C:751:THR:HA	3:C:754:ILE:HG22	1.98	0.45
1:D:125:ARG:NH1	1:D:195:GLU:HA	2.32	0.45
2:E:309:TRP:HZ2	2:E:416:SER:HB3	1.81	0.45
3:F:599:LEU:HA	3:F:599:LEU:HD23	1.84	0.45
1:G:205:PHE:H	2:H:332:TRP:HB3	1.81	0.45
3:I:550:TYR:O	3:I:554:ILE:HG13	2.15	0.45
1:J:179:ARG:HG2	1:J:188:TRP:CZ3	2.50	0.45
3:L:118:TYR:OH	3:L:206:MET:SD	2.64	0.45
3:L:423:ARG:H	3:L:423:ARG:HD2	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:89:THR:HG21	3:L:755:ARG:NH1	2.32	0.45
2:B:318:PHE:HD1	2:B:415:LEU:HD23	1.82	0.45
2:B:666:TRP:CB	3:C:58:THR:HG22	2.47	0.45
3:C:407:GLU:OE2	3:C:476:ARG:NH1	2.49	0.45
3:C:71:ASN:OD1	3:C:74:GLY:N	2.49	0.45
3:F:459:GLY:O	3:F:482:LYS:HB2	2.16	0.45
3:I:275:ASP:CB	1:J:96:ASN:HD21	2.25	0.45
2:K:697:GLU:OE2	3:L:32:LYS:NZ	2.34	0.45
1:A:710:PHE:O	1:A:714:ALA:N	2.50	0.45
3:C:504:VAL:HG21	3:C:513:LEU:HB2	1.99	0.45
3:C:753:ARG:HA	3:C:753:ARG:HD2	1.74	0.45
2:E:285:VAL:O	2:E:289:MET:HG2	2.17	0.45
2:E:316:ARG:HG2	2:E:316:ARG:H	1.59	0.45
2:E:78:GLU:O	2:E:471:LYS:NZ	2.46	0.45
1:A:57:ARG:HB3	3:F:628:GLN:HA	1.98	0.45
1:A:210:THR:H	1:A:213:ARG:HD3	1.80	0.45
1:A:491:THR:HG22	1:A:497:LYS:HE3	1.99	0.45
1:A:446:PHE:CE1	1:A:637:CYS:HB3	2.52	0.45
1:A:583:ARG:HD3	2:B:25:THR:HG21	1.99	0.45
2:B:273:VAL:HB	2:B:277:GLU:HG3	1.98	0.45
2:E:84:GLN:O	2:E:88:VAL:HG23	2.16	0.45
3:F:333:THR:HB	3:F:362:GLU:O	2.17	0.45
3:F:499:ASP:OD2	3:F:503:ARG:HB2	2.15	0.45
3:F:60:ASP:HB2	3:F:62:ARG:HH21	1.81	0.45
1:G:431:ASP:O	1:G:437:HIS:NE2	2.50	0.45
1:G:217:GLN:NE2	2:H:58:ASN:HA	2.22	0.45
1:G:432:VAL:HG11	2:H:602:ARG:HD3	1.99	0.45
3:I:141:ILE:HG21	3:I:143:ARG:HH21	1.80	0.45
3:I:395:ALA:O	3:I:398:ILE:HG22	2.16	0.45
3:I:537:TRP:CE3	3:I:545:VAL:HG13	2.51	0.45
1:J:305:TYR:OH	1:J:354:ILE:HG22	2.16	0.45
1:J:362:LYS:HB3	1:J:367:LYS:HE3	1.99	0.45
1:J:431:ASP:HB3	1:J:437:HIS:HD2	1.82	0.45
1:A:280:SER:HB3	1:A:650:TYR:CZ	2.51	0.45
1:A:75:ARG:NH1	1:A:111:ASP:OD2	2.50	0.45
3:C:395:ALA:O	3:C:399:ILE:HG12	2.16	0.45
1:D:530:PRO:HB3	1:D:564:TYR:HE1	1.81	0.45
1:D:53:PHE:CE2	1:D:63:VAL:HG21	2.52	0.45
3:F:337:SER:OG	3:F:361:GLU:OE1	2.20	0.45
3:F:77:LEU:O	3:F:78:TRP:HD1	2.00	0.45
1:G:328:LYS:HA	1:G:328:LYS:HD3	1.78	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:287:ARG:O	2:H:291:THR:OG1	2.35	0.45
2:H:514:VAL:HG22	2:H:516:GLY:H	1.80	0.45
1:J:420:SER:HB3	1:J:489:CYS:HB2	1.98	0.45
1:J:583:ARG:NH1	2:K:509:LEU:HG	2.31	0.45
2:K:605:HIS:CD2	2:K:606:ILE:HG13	2.51	0.45
1:A:179:ARG:HG2	1:A:188:TRP:CZ3	2.52	0.45
1:A:359:ASN:ND2	1:A:479:ASP:OD2	2.50	0.45
1:A:568:ASN:OD1	1:A:569:GLY:N	2.40	0.45
3:C:270:ALA:O	3:C:276:PRO:HB3	2.17	0.45
3:C:318:ARG:HD3	3:C:493:ARG:HB3	1.99	0.45
3:C:619:LEU:O	3:C:622:THR:HG23	2.17	0.45
1:D:478:ASP:OD1	1:D:510:HIS:HE1	1.99	0.45
1:D:54:ILE:HA	1:D:60:SER:HA	1.99	0.45
2:E:254:PHE:O	2:E:257:THR:OG1	2.30	0.45
3:F:79:SER:OG	3:F:80:LYS:N	2.49	0.45
1:G:326:HIS:O	1:G:326:HIS:ND1	2.50	0.45
2:H:586:LYS:O	2:H:589:LEU:HD12	2.16	0.45
3:I:589:ARG:HG2	3:I:624:ALA:HB2	1.99	0.45
3:I:752:LYS:HA	3:I:752:LYS:HD3	1.72	0.45
2:K:155:LEU:HD12	2:K:155:LEU:H	1.81	0.45
1:A:455:ALA:HA	1:A:458:TYR:CD2	2.52	0.45
1:A:537:TRP:HB3	1:A:540:TYR:HB2	1.98	0.45
2:B:160:SER:O	3:C:27:HIS:NE2	2.50	0.45
2:B:565:ASP:HB2	2:B:580:TRP:CH2	2.52	0.45
2:B:58:ASN:ND2	2:B:65:GLN:OE1	2.36	0.45
3:C:610:PHE:HD2	3:C:615:ILE:HD11	1.81	0.45
2:E:77:HIS:O	2:E:77:HIS:ND1	2.47	0.45
2:E:280:ALA:HB3	3:F:142:ARG:HD3	1.99	0.45
1:G:369:ALA:HB1	1:G:521:VAL:HG21	1.99	0.45
2:H:574:PHE:HZ	2:H:578:LYS:HZ3	1.65	0.45
3:I:212:VAL:HG12	3:I:213:ARG:O	2.16	0.45
2:H:696:PHE:CD2	3:I:28:ILE:HG12	2.51	0.45
3:I:535:MET:CG	3:I:536:MET:H	2.30	0.45
1:J:249:MET:SD	2:K:468:ARG:NE	2.90	0.45
1:J:401:ARG:HH11	1:J:696:ASN:HB2	1.82	0.45
2:K:170:VAL:O	2:K:173:SER:OG	2.35	0.45
2:K:349:ALA:HB3	2:K:401:ALA:HB3	1.99	0.45
2:K:419:LEU:O	2:K:422:SER:OG	2.26	0.45
3:L:638:VAL:HG23	3:L:645:MET:HB2	1.98	0.45
1:A:654:GLN:HE22	1:A:695:ILE:HB	1.82	0.45
2:B:112:GLU:HG2	2:B:116:GLN:NE2	2.26	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:410:GLY:H	2:B:413:ASN:HD21	1.63	0.45
1:D:217:GLN:HE22	2:E:58:ASN:HA	1.81	0.45
3:I:28:ILE:HA	3:I:31:ILE:HG22	1.98	0.45
3:I:139:VAL:HG23	3:I:483:MET:HE3	1.98	0.45
2:K:112:GLU:HG2	2:K:116:GLN:OE1	2.17	0.45
2:K:137:GLN:OE1	2:K:141:THR:HG21	2.16	0.45
2:K:626:ASN:HB3	3:L:99:TRP:HH2	1.81	0.45
3:L:504:VAL:HG12	3:L:512:LEU:HD12	1.99	0.45
3:L:752:LYS:HD3	3:L:752:LYS:HA	1.72	0.45
1:A:477:MET:HA	1:A:509:SER:OG	2.16	0.44
2:B:268:GLN:HB2	2:B:421:VAL:HG13	1.99	0.44
2:B:519:GLU:O	2:B:555:TYR:OH	2.21	0.44
2:B:70:ASP:HA	2:B:84:GLN:HA	1.98	0.44
3:C:116:LYS:HE2	3:C:120:GLU:OE2	2.17	0.44
3:C:429:ASN:N	3:C:429:ASN:OD1	2.50	0.44
1:D:111:ASP:HB3	1:D:116:ARG:H	1.82	0.44
1:D:681:PHE:CZ	2:E:484:ILE:HD11	2.52	0.44
3:F:176:ILE:HG22	3:F:693:GLY:HA3	1.99	0.44
1:G:431:ASP:OD2	1:G:440:SER:HB2	2.17	0.44
1:G:316:GLY:O	1:G:546:GLY:HA3	2.17	0.44
1:G:657:GLY:O	1:G:661:GLU:HG2	2.17	0.44
2:H:605:HIS:HB3	3:I:233:HIS:HE1	1.81	0.44
3:I:736:LYS:NZ	3:I:737:ARG:O	2.38	0.44
1:J:587:GLN:O	1:J:591:GLN:NE2	2.39	0.44
3:L:498:ILE:HD11	3:L:502:LEU:HA	1.98	0.44
1:A:298:GLU:O	1:A:300:GLU:N	2.51	0.44
3:C:449:TRP:NE1	3:C:476:ARG:HB3	2.24	0.44
3:F:141:ILE:HG21	3:F:143:ARG:HH21	1.82	0.44
1:G:78:ILE:HA	1:G:109:LEU:HD12	1.98	0.44
2:H:316:ARG:H	2:H:316:ARG:HG2	1.55	0.44
2:H:151:ARG:NE	3:I:18:GLU:OE1	2.48	0.44
3:I:39:GLN:HG2	3:I:39:GLN:H	1.61	0.44
3:I:452:GLU:OE2	3:I:477:GLY:N	2.44	0.44
1:J:254:ASN:HB2	2:K:464:ASP:OD2	2.16	0.44
1:J:283:LEU:O	1:J:461:LYS:NZ	2.50	0.44
1:J:641:LEU:O	1:J:645:VAL:HG23	2.17	0.44
2:K:666:TRP:HB3	3:L:58:THR:HG22	1.99	0.44
3:L:341:GLU:HG3	3:L:355:ARG:HA	2.00	0.44
3:L:365:MET:HE3	3:L:372:ALA:HB3	1.98	0.44
1:A:530:PRO:HB3	1:A:564:TYR:HE1	1.82	0.44
1:D:455:ALA:O	1:D:459:ILE:HG13	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:144:HIS:CE1	1:G:157:THR:H	2.35	0.44
3:I:121:LYS:HA	3:I:124:ARG:HD2	1.99	0.44
3:I:189:LYS:HA	3:I:189:LYS:HD3	1.77	0.44
1:J:179:ARG:NH1	2:K:711:ILE:HG13	2.33	0.44
2:K:70:ASP:HA	2:K:84:GLN:HA	1.99	0.44
3:L:142:ARG:HB3	3:L:217:PHE:HE1	1.82	0.44
3:L:220:VAL:HG12	3:L:223:GLY:H	1.82	0.44
3:L:260:ILE:O	3:L:264:ARG:HG3	2.18	0.44
3:L:456:ASN:ND2	3:L:471:THR:O	2.51	0.44
2:K:724:ILE:HG21	3:L:709:SER:HB2	1.99	0.44
1:A:362:LYS:HB3	1:A:367:LYS:HE3	1.99	0.44
1:A:529:ASP:OD1	1:A:529:ASP:N	2.50	0.44
2:B:86:ASP:O	2:B:90:GLU:HB2	2.17	0.44
3:C:382:ILE:HA	3:C:382:ILE:HD13	1.92	0.44
1:D:124:ARG:HG3	1:D:150:PHE:CE1	2.52	0.44
1:D:431:ASP:O	1:D:437:HIS:NE2	2.50	0.44
3:F:382:ILE:HA	3:F:382:ILE:HD13	1.90	0.44
1:G:174:ARG:HE	1:G:178:ILE:HD11	1.82	0.44
2:H:15:GLN:HB2	2:H:498:ARG:HD2	2.00	0.44
3:I:230:GLU:HG3	3:I:231:VAL:HG13	1.98	0.44
1:A:420:SER:HB3	1:A:489:CYS:HB2	1.99	0.44
3:C:142:ARG:HB3	3:C:217:PHE:CE1	2.52	0.44
3:C:372:ALA:HA	3:C:385:ILE:O	2.16	0.44
3:F:463:ILE:HD11	3:F:467:MET:HA	1.98	0.44
1:G:384:CYS:HB2	1:G:387:VAL:HG21	1.97	0.44
1:G:455:ALA:HA	1:G:458:TYR:CD2	2.52	0.44
1:G:606:ASP:HB2	3:I:135:PHE:CD2	2.52	0.44
1:J:278:GLN:HG2	1:J:280:SER:H	1.83	0.44
1:J:469:LEU:O	1:J:473:SER:OG	2.33	0.44
2:K:469:THR:HA	2:K:472:LEU:HD12	1.98	0.44
3:L:360:TYR:CE1	3:L:375:ARG:HB3	2.53	0.44
2:B:671:ASN:ND2	3:C:38:ARG:HH22	2.16	0.44
3:C:395:ALA:O	3:C:398:ILE:HG22	2.17	0.44
3:C:499:ASP:OD2	3:C:503:ARG:HB2	2.18	0.44
2:E:104:GLU:OE2	2:E:327:ARG:N	2.50	0.44
2:E:750:ILE:HD13	3:F:4:ILE:HD11	1.98	0.44
3:F:589:ARG:HG2	3:F:624:ALA:HB2	1.99	0.44
2:H:485:ASN:N	2:H:485:ASN:OD1	2.50	0.44
2:H:520:SER:OG	2:H:662:THR:HG21	2.17	0.44
3:I:339:LYS:HG3	3:I:340:LYS:H	1.83	0.44
2:K:470:CYS:HB3	2:K:475:ILE:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:689:TYR:HD1	3:L:31:ILE:HD11	1.82	0.44
3:L:251:ARG:O	3:L:255:VAL:HG23	2.17	0.44
3:L:55:TYR:H	3:L:92:SER:HB2	1.81	0.44
2:B:80:SER:N	2:B:476:ASN:OD1	2.34	0.44
1:A:606:ASP:HB2	3:C:135:PHE:CD2	2.51	0.44
1:D:111:ASP:OD1	1:D:113:LYS:N	2.51	0.44
1:D:75:ARG:HG3	1:D:76:PHE:CD2	2.53	0.44
2:E:467:TYR:OH	2:E:471:LYS:HE3	2.18	0.44
3:F:597:ARG:NH2	3:F:624:ALA:O	2.50	0.44
1:G:706:TRP:CD2	2:H:5:PRO:HD2	2.53	0.44
2:H:605:HIS:HD2	3:I:233:HIS:NE2	2.16	0.44
2:H:692:CYS:SG	3:I:20:LEU:HD21	2.57	0.44
3:I:146:ASP:HA	3:I:215:THR:HA	1.99	0.44
2:K:217:TYR:HD2	2:K:218:LEU:HD12	1.83	0.44
2:K:696:PHE:HE2	2:K:703:SER:HB3	1.80	0.44
1:A:418:THR:HG21	1:A:454:ARG:HD3	2.00	0.44
1:A:72:LEU:O	1:A:74:HIS:ND1	2.48	0.44
2:B:163:LEU:O	2:B:167:LEU:HG	2.17	0.44
2:B:456:HIS:HA	2:B:459:ILE:HD11	2.00	0.44
1:D:477:MET:HG2	1:D:510:HIS:CE1	2.52	0.44
1:G:108:ASP:HB2	1:G:119:GLU:HA	2.00	0.44
1:J:283:LEU:HG	1:J:524:GLU:HG2	1.99	0.44
2:K:298:LEU:HB2	2:K:453:ALA:O	2.18	0.44
2:K:531:LYS:NZ	2:K:532:ASN:OD1	2.40	0.44
2:K:276:ASN:ND2	2:K:535:ILE:O	2.47	0.44
2:K:68:PRO:HD2	2:K:314:ASN:HD21	1.83	0.44
3:L:124:ARG:HB3	3:L:246:PRO:HB2	1.98	0.44
3:L:462:GLY:O	3:L:469:PRO:HA	2.17	0.44
3:L:600:PHE:CZ	3:L:619:LEU:HA	2.52	0.44
2:B:413:ASN:HB3	2:B:444:SER:OG	2.17	0.44
2:B:492:PHE:O	2:B:495:PHE:HB2	2.18	0.44
2:B:669:LYS:HA	2:B:669:LYS:HD3	1.84	0.44
3:C:135:PHE:CE2	3:C:240:TRP:HB3	2.53	0.44
3:C:694:PHE:HB3	3:C:734:VAL:HG13	1.99	0.44
2:E:224:LEU:HD12	2:E:224:LEU:HA	1.74	0.44
3:F:163:ILE:O	3:F:167:VAL:HG12	2.17	0.44
3:F:70:ARG:CG	3:F:74:GLY:HA2	2.48	0.44
2:H:578:LYS:HE3	3:I:101:ARG:NH1	2.33	0.44
3:L:581:GLN:OE1	3:L:589:ARG:NH1	2.51	0.44
1:A:125:ARG:HG2	1:A:126:GLU:H	1.83	0.43
1:A:470:LEU:HG	3:C:49:TRP:HZ2	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:523:MET:HB3	1:A:563:LEU:HD21	2.00	0.43
1:A:556:GLN:OE1	1:A:556:GLN:N	2.51	0.43
2:B:378:LEU:HD21	2:B:389:ILE:HG22	1.99	0.43
2:B:567:GLN:HA	2:B:577:LYS:NZ	2.33	0.43
1:D:588:SER:O	1:D:591:GLN:HG2	2.17	0.43
2:H:559:TYR:HE2	2:H:664:HIS:HD2	1.64	0.43
1:J:41:HIS:CE1	1:J:120:ILE:HB	2.53	0.43
2:K:157:ALA:HB1	2:K:165:ASP:HB3	1.99	0.43
1:A:290:LEU:O	1:A:292:ILE:HG13	2.17	0.43
1:A:482:LEU:HD11	1:A:503:PHE:HD2	1.83	0.43
2:B:215:LYS:O	2:B:219:ILE:HG13	2.18	0.43
2:B:464:ASP:O	2:B:468:ARG:HG2	2.18	0.43
1:D:261:LEU:O	1:D:265:PRO:HD3	2.18	0.43
1:D:477:MET:HG2	1:D:510:HIS:ND1	2.32	0.43
1:D:210:THR:OG1	2:E:175:ASP:HA	2.17	0.43
1:G:261:LEU:O	1:G:264:THR:OG1	2.33	0.43
3:I:387:SER:HB3	3:I:485:VAL:HG23	2.01	0.43
1:J:446:PHE:O	1:J:450:VAL:HG23	2.18	0.43
2:K:746:ILE:O	2:K:750:ILE:HG13	2.18	0.43
1:A:189:ASP:HA	2:B:162:ARG:NH1	2.33	0.43
3:C:298:LEU:HD22	3:C:312:LYS:HG3	2.00	0.43
3:C:318:ARG:NH1	3:C:493:ARG:O	2.42	0.43
2:E:410:GLY:N	2:E:413:ASN:HD21	2.13	0.43
2:E:427:GLY:HA3	2:E:438:TRP:CE2	2.53	0.43
3:F:541:GLY:HA3	3:F:641:ARG:NH1	2.33	0.43
3:F:55:TYR:H	3:F:92:SER:HB2	1.83	0.43
3:F:712:GLU:HB3	3:F:715:ASN:HD21	1.83	0.43
3:I:265:ASN:OD1	3:I:268:ARG:NH1	2.50	0.43
1:J:41:HIS:HE1	1:J:120:ILE:HB	1.82	0.43
1:J:443:ARG:HG3	1:J:444:ASN:N	2.32	0.43
1:J:73:LYS:HD2	1:J:73:LYS:HA	1.66	0.43
2:K:211:ARG:HA	2:K:211:ARG:HD2	1.79	0.43
2:K:249:ARG:O	2:K:252:VAL:HG12	2.18	0.43
2:K:421:VAL:HA	2:K:424:LEU:HD12	2.00	0.43
2:K:527:VAL:HG11	2:K:599:TYR:CD2	2.53	0.43
2:K:276:ASN:CB	3:L:219:PRO:HG3	2.46	0.43
1:A:583:ARG:NH2	2:B:511:SER:HA	2.32	0.43
3:C:368:ARG:HG2	3:C:368:ARG:H	1.51	0.43
1:D:484:PRO:HB2	1:D:486:ILE:HG13	1.99	0.43
1:D:513:ASN:HB2	1:D:516:ASP:OD1	2.19	0.43
1:D:74:HIS:C	1:D:76:PHE:H	2.22	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:601:ILE:HA	2:E:604:LEU:HG	2.00	0.43
3:F:704:TYR:CG	3:F:721:LYS:NZ	2.61	0.43
3:F:61:LYS:NZ	3:F:87:ASP:OD1	2.51	0.43
2:H:167:LEU:HD13	2:H:251:PHE:CE1	2.53	0.43
2:H:276:ASN:O	2:H:279:LYS:HB2	2.18	0.43
1:J:154:GLU:OE1	1:J:172:LYS:NZ	2.40	0.43
1:J:72:LEU:O	1:J:74:HIS:ND1	2.51	0.43
2:K:215:LYS:HE2	2:K:215:LYS:HB3	1.88	0.43
2:K:420:GLY:HA3	2:K:442:GLN:HG2	2.00	0.43
2:K:528:THR:O	2:K:531:LYS:HG2	2.18	0.43
1:A:483:ILE:HB	1:A:504:ILE:HB	2.01	0.43
1:A:513:ASN:N	1:A:516:ASP:OD2	2.41	0.43
1:A:641:LEU:O	1:A:645:VAL:HG23	2.17	0.43
1:A:663:ARG:HG3	2:B:18:ILE:HD11	2.01	0.43
2:B:316:ARG:HG2	2:B:316:ARG:H	1.60	0.43
2:B:407:MET:HE3	2:B:412:PHE:H	1.84	0.43
2:B:423:ILE:HA	2:B:423:ILE:HD12	1.91	0.43
2:B:504:ASN:OD1	2:B:507:MET:HG3	2.18	0.43
2:B:550:LEU:HD23	2:B:550:LEU:HA	1.83	0.43
1:D:381:PHE:CE1	1:D:385:LYS:HD2	2.52	0.43
1:D:287:ALA:HA	1:D:525:PHE:O	2.18	0.43
2:E:524:SER:OG	2:E:657:TYR:HD2	2.00	0.43
2:E:686:GLU:HG2	2:E:686:GLU:O	2.19	0.43
3:I:753:ARG:HA	3:I:753:ARG:HD2	1.66	0.43
2:H:572:ARG:HG3	3:I:94:LEU:HG	1.99	0.43
1:J:258:GLU:OE2	1:J:683:LEU:N	2.52	0.43
3:L:315:MET:HE2	3:L:315:MET:HB3	1.91	0.43
3:L:286:SER:OG	3:L:533:SER:HB3	2.18	0.43
1:A:125:ARG:HH11	1:A:195:GLU:HA	1.83	0.43
1:A:654:GLN:OE1	1:A:695:ILE:N	2.43	0.43
2:B:303:THR:HG21	2:B:491:GLU:HB3	1.99	0.43
3:C:554:ILE:HG21	3:C:673:GLY:HA3	1.99	0.43
2:E:389:ILE:HA	2:E:392:ILE:HG22	2.01	0.43
3:F:189:LYS:O	3:F:193:LEU:HG	2.18	0.43
3:I:375:ARG:HB2	3:I:382:ILE:O	2.19	0.43
3:I:67:ILE:HG13	3:I:78:TRP:HZ2	1.83	0.43
2:K:309:TRP:CD1	2:K:310:ASN:N	2.86	0.43
2:K:330:PRO:O	2:K:334:ARG:HG3	2.18	0.43
3:L:121:LYS:HA	3:L:124:ARG:HD2	2.01	0.43
3:C:13:GLN:O	3:C:16:THR:OG1	2.37	0.43
2:B:671:ASN:ND2	3:C:38:ARG:HH12	2.16	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:307:ALA:HB1	1:D:500:LEU:HD22	2.01	0.43
1:D:655:LEU:HD22	1:D:699:TRP:HD1	1.83	0.43
2:E:99:HIS:HA	2:E:100:PRO:HD3	1.84	0.43
2:E:750:ILE:O	2:E:754:ARG:N	2.46	0.43
3:F:395:ALA:O	3:F:399:ILE:HG12	2.19	0.43
3:F:619:LEU:O	3:F:621:PHE:N	2.52	0.43
2:H:494:SER:HB2	2:H:505:PHE:HA	2.00	0.43
2:H:690:GLN:OE1	3:I:35:THR:OG1	2.22	0.43
1:J:292:ILE:HD12	1:J:498:THR:HB	2.01	0.43
1:J:603:LYS:HD3	1:J:603:LYS:HA	1.76	0.43
2:K:711:ILE:O	3:L:24:THR:OG1	2.24	0.43
3:L:225:SER:O	3:L:229:ILE:HG12	2.18	0.43
3:L:281:LEU:HD21	3:L:314:ALA:HB1	2.00	0.43
3:L:269:ARG:NH2	3:L:535:MET:HG3	2.34	0.43
1:A:52:HIS:CD2	1:A:163:LEU:HD21	2.53	0.43
1:A:314:PHE:HD2	1:A:317:TRP:CE2	2.36	0.43
1:A:618:THR:HB	1:A:630:GLU:HB3	2.00	0.43
2:B:24:TYR:HE2	2:B:28:PRO:HG3	1.83	0.43
3:C:326:GLY:N	3:C:517:GLU:OE1	2.52	0.43
3:C:576:GLU:OE1	3:C:576:GLU:N	2.52	0.43
2:E:599:TYR:OH	2:E:608:GLU:N	2.52	0.43
1:G:335:LEU:HD12	1:G:336:LEU:HD12	2.01	0.43
1:G:431:ASP:HB3	1:G:437:HIS:HD2	1.84	0.43
2:H:279:LYS:HD3	2:H:501:PHE:CD2	2.54	0.43
2:H:708:PRO:HD2	3:I:28:ILE:HG22	2.00	0.43
3:I:465:PRO:HD3	3:I:475:LEU:HD21	2.00	0.43
3:I:478:VAL:O	3:I:479:ARG:NH1	2.41	0.43
2:K:267:GLU:OE1	2:K:281:LYS:HG2	2.19	0.43
2:K:306:ASN:OD1	2:K:477:MET:HA	2.19	0.43
1:J:664:ARG:NH2	2:K:446:ASP:OD2	2.48	0.43
2:K:506:SER:HB3	2:K:537:ASN:OD1	2.18	0.43
2:K:120:ASP:HB3	3:L:33:LYS:HD2	2.01	0.43
3:L:144:ARG:NE	3:L:489:SER:O	2.44	0.43
1:A:123:THR:HG21	1:A:130:TYR:CG	2.54	0.43
1:A:370:LEU:HD13	1:A:507:GLY:HA2	2.00	0.43
2:B:167:LEU:HD22	2:B:251:PHE:CZ	2.54	0.43
3:C:116:LYS:HG2	3:C:120:GLU:HG3	2.01	0.43
3:C:611:ASP:O	3:C:615:ILE:HG13	2.19	0.43
2:E:306:ASN:OD1	2:E:477:MET:HA	2.18	0.43
3:F:432:HIS:O	3:F:436:ARG:HG2	2.19	0.43
1:G:253:VAL:O	2:H:468:ARG:HD3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:48:GLN:O	2:H:51:GLU:HG2	2.19	0.43
3:I:312:LYS:O	3:I:317:LEU:HB2	2.19	0.43
1:J:590:GLN:HG3	1:J:591:GLN:N	2.33	0.43
3:L:362:GLU:HG3	3:L:375:ARG:HG2	2.01	0.43
1:A:431:ASP:OD2	1:A:440:SER:HB2	2.19	0.43
1:A:597:GLU:O	1:A:601:SER:N	2.51	0.43
3:C:298:LEU:HB3	3:C:312:LYS:HG2	2.00	0.43
3:C:334:SER:OG	3:C:362:GLU:HB3	2.18	0.43
1:D:418:THR:CG2	1:D:454:ARG:HD3	2.48	0.43
1:D:425:LEU:HD12	1:D:425:LEU:HA	1.80	0.43
1:D:576:LYS:HA	1:D:579:MET:HG3	2.00	0.43
2:E:222:LEU:HD13	2:E:346:ASN:O	2.19	0.43
1:G:571:SER:H	1:G:574:LYS:HB2	1.84	0.43
2:H:224:LEU:N	2:H:348:MET:O	2.51	0.43
2:H:518:ASN:OD1	2:H:520:SER:N	2.51	0.43
2:H:698:LYS:HE2	2:H:698:LYS:HB2	1.71	0.43
1:J:491:THR:OG1	1:J:495:ARG:N	2.47	0.43
1:A:256:ARG:HG2	1:A:256:ARG:H	1.58	0.42
1:D:477:MET:O	1:D:510:HIS:ND1	2.51	0.42
1:G:111:ASP:OD1	1:G:113:LYS:N	2.52	0.42
2:H:457:GLU:N	2:H:457:GLU:OE1	2.52	0.42
3:I:11:MET:SD	3:I:17:ARG:HA	2.58	0.42
2:K:565:ASP:HB2	2:K:580:TRP:CZ2	2.54	0.42
2:K:586:LYS:O	2:K:589:LEU:HD12	2.19	0.42
1:A:713:HIS:O	2:B:10:LEU:HD11	2.19	0.42
2:B:271:LEU:HD11	2:B:443:SER:HA	1.99	0.42
2:B:309:TRP:CZ2	2:B:416:SER:HB3	2.52	0.42
3:C:407:GLU:OE1	3:C:476:ARG:NH2	2.52	0.42
2:E:347:LYS:HZ1	2:E:406:GLY:N	2.17	0.42
2:E:457:GLU:N	2:E:457:GLU:OE1	2.52	0.42
3:F:384:LEU:O	3:F:479:ARG:N	2.53	0.42
3:F:746:ASP:O	3:F:749:THR:OG1	2.13	0.42
1:G:338:TRP:NE1	1:G:545:ILE:HD11	2.34	0.42
1:G:577:TRP:HZ2	1:G:648:SER:HA	1.84	0.42
2:H:605:HIS:HD2	3:I:233:HIS:CE1	2.37	0.42
1:J:130:TYR:CE1	1:J:197:GLY:HA2	2.53	0.42
1:J:363:THR:HB	1:J:365:GLN:OE1	2.19	0.42
1:J:504:ILE:HA	1:J:521:VAL:O	2.19	0.42
2:K:110:THR:O	2:K:114:VAL:HG13	2.19	0.42
2:K:689:TYR:CG	3:L:34:TYR:HD2	2.36	0.42
2:B:582:GLN:OE1	3:C:101:ARG:HD2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:387:SER:HB3	3:C:485:VAL:HG23	2.00	0.42
3:C:506:ASP:CG	3:C:512:LEU:HD11	2.39	0.42
1:D:328:LYS:HD3	1:D:328:LYS:HA	1.91	0.42
1:D:500:LEU:HD21	1:D:503:PHE:CE1	2.50	0.42
1:D:545:ILE:HG22	1:D:561:MET:O	2.19	0.42
2:E:305:ASP:HB2	2:E:446:ASP:OD1	2.19	0.42
2:E:330:PRO:O	2:E:334:ARG:HG3	2.19	0.42
3:F:534:SER:O	3:F:536:MET:N	2.52	0.42
3:I:225:SER:OG	3:I:226:SER:N	2.52	0.42
2:K:99:HIS:HA	2:K:100:PRO:HD3	1.84	0.42
1:A:166:GLU:OE2	3:C:738:LYS:N	2.52	0.42
1:A:154:GLU:OE1	1:A:168:ARG:NH1	2.52	0.42
1:A:454:ARG:HG2	1:A:458:TYR:CZ	2.54	0.42
1:A:60:SER:CB	1:A:75:ARG:HE	2.31	0.42
1:A:82:ARG:HG2	3:C:754:ILE:CD1	2.49	0.42
3:C:264:ARG:HH22	3:C:368:ARG:NH1	2.17	0.42
3:C:544:SER:HA	3:C:547:VAL:HG22	2.01	0.42
3:F:429:ASN:N	3:F:429:ASN:OD1	2.50	0.42
3:F:535:MET:SD	3:F:535:MET:N	2.93	0.42
1:G:68:PRO:HA	1:G:71:LEU:O	2.20	0.42
2:H:114:VAL:HG12	2:H:254:PHE:CE1	2.55	0.42
3:I:141:ILE:HG22	3:I:143:ARG:HB2	2.00	0.42
1:J:366:LEU:HD21	1:J:505:ILE:HG21	2.00	0.42
1:J:466:ASN:HB2	1:J:579:MET:HG2	2.02	0.42
2:K:111:MET:HG2	2:K:333:PHE:CD1	2.53	0.42
1:A:125:ARG:HH21	1:A:129:ILE:HG22	1.85	0.42
1:A:435:ILE:O	1:A:438:ILE:N	2.52	0.42
2:B:140:ALA:HB3	3:C:35:THR:O	2.19	0.42
2:B:708:PRO:HA	3:C:728:GLN:HE21	1.84	0.42
1:D:269:ARG:HD3	1:D:691:GLU:OE1	2.19	0.42
2:E:107:CYS:SG	2:E:325:ILE:HG22	2.60	0.42
1:G:596:ILE:HG12	1:G:611:PHE:CD2	2.54	0.42
2:H:516:GLY:N	2:H:522:ASP:OD1	2.53	0.42
2:H:693:CYS:SG	3:I:31:ILE:HG23	2.60	0.42
3:I:235:THR:O	3:I:241:GLU:HA	2.20	0.42
1:J:427:GLU:OE2	1:J:427:GLU:N	2.49	0.42
2:K:601:ILE:HA	2:K:604:LEU:HG	2.02	0.42
1:A:179:ARG:HD3	2:B:711:ILE:HD11	2.02	0.42
1:D:422:TRP:CE3	1:D:489:CYS:HB3	2.54	0.42
2:E:215:LYS:O	2:E:219:ILE:HG13	2.19	0.42
2:E:58:ASN:OD1	2:E:60:GLU:N	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:197:LYS:H	3:F:197:LYS:HG2	1.68	0.42
1:G:171:ILE:O	1:G:175:LEU:HG	2.19	0.42
1:G:530:PRO:HG3	1:G:542:VAL:HG11	2.02	0.42
2:H:258:LEU:O	2:H:262:ILE:N	2.52	0.42
2:H:550:LEU:HD23	2:H:550:LEU:HA	1.80	0.42
1:J:54:ILE:HD11	1:J:75:ARG:HD3	2.01	0.42
3:L:325:PHE:O	3:L:328:PHE:HB2	2.20	0.42
2:K:140:ALA:HB3	3:L:35:THR:O	2.20	0.42
3:L:436:ARG:HA	3:L:436:ARG:HD3	1.90	0.42
3:L:754:ILE:HG13	3:L:755:ARG:HG2	2.01	0.42
3:C:454:ILE:HG12	3:C:472:GLU:C	2.40	0.42
3:C:67:ILE:HG22	3:C:98:TRP:HZ3	1.83	0.42
1:D:457:GLU:OE2	1:D:501:TYR:OH	2.17	0.42
2:E:58:ASN:HB2	2:E:63:ALA:O	2.19	0.42
3:F:141:ILE:HG21	3:F:143:ARG:HE	1.84	0.42
3:F:541:GLY:O	3:F:544:SER:OG	2.23	0.42
1:D:166:GLU:OE2	3:F:738:LYS:HB2	2.19	0.42
3:F:71:ASN:OD1	3:F:74:GLY:N	2.53	0.42
2:H:258:LEU:O	2:H:262:ILE:HG13	2.20	0.42
2:H:378:LEU:HD11	2:H:389:ILE:HG21	2.01	0.42
2:H:635:LYS:HA	2:H:635:LYS:HD3	1.72	0.42
3:I:554:ILE:HG23	3:I:675:LEU:HD11	2.02	0.42
1:J:5:VAL:O	1:J:9:PHE:HD2	2.03	0.42
2:K:667:ILE:HG23	3:L:50:MET:HE1	2.02	0.42
1:A:28:PRO:HB3	1:A:35:PHE:CD2	2.55	0.42
1:A:432:VAL:HG22	1:A:436:GLU:CD	2.40	0.42
1:A:69:ASN:O	1:A:69:ASN:ND2	2.53	0.42
2:B:289:MET:O	2:B:452:ASN:ND2	2.52	0.42
3:C:289:ILE:HD13	3:C:294:MET:HB2	2.02	0.42
1:D:305:TYR:OH	1:D:354:ILE:HG22	2.20	0.42
3:F:288:GLN:HB2	3:F:530:THR:HB	2.01	0.42
3:F:617:LYS:HE3	3:F:649:VAL:HA	2.01	0.42
1:G:305:TYR:OH	1:G:354:ILE:HG22	2.19	0.42
1:G:500:LEU:HD21	1:G:503:PHE:CE1	2.55	0.42
1:G:513:ASN:N	1:G:516:ASP:OD2	2.43	0.42
2:H:268:GLN:NE2	2:H:439:ASP:OD1	2.53	0.42
2:H:735:ILE:HA	2:H:735:ILE:HD12	1.89	0.42
3:I:346:THR:HB	3:I:414:VAL:HG11	2.01	0.42
1:J:455:ALA:O	1:J:459:ILE:HG13	2.19	0.42
1:J:422:TRP:CE2	1:J:457:GLU:HB2	2.55	0.42
2:K:599:TYR:OH	2:K:608:GLU:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:570:MET:HB3	3:L:570:MET:HE3	1.88	0.42
3:L:619:LEU:O	3:L:622:THR:HG23	2.20	0.42
1:A:179:ARG:HG2	1:A:188:TRP:HZ3	1.85	0.42
2:B:598:LEU:H	2:B:598:LEU:HD23	1.85	0.42
3:C:111:TYR:O	3:C:113:LYS:N	2.42	0.42
2:B:575:GLU:OE1	3:C:98:TRP:HD1	2.03	0.42
1:D:584:CYS:O	1:D:588:SER:OG	2.28	0.42
2:E:277:GLU:OE2	3:F:219:PRO:HD3	2.20	0.42
3:F:506:ASP:OD1	3:F:506:ASP:N	2.53	0.42
1:G:587:GLN:HG2	1:G:591:GLN:HE22	1.84	0.42
1:J:359:ASN:HA	1:J:480:PHE:O	2.20	0.42
2:K:167:LEU:HD13	2:K:251:PHE:CE1	2.55	0.42
2:K:65:GLN:NE2	2:K:346:ASN:OD1	2.34	0.42
2:K:449:LEU:HG	2:K:450:ILE:N	2.33	0.42
3:L:120:GLU:HB3	3:L:124:ARG:CZ	2.49	0.42
1:A:587:GLN:HG2	1:A:591:GLN:HE21	1.85	0.42
1:A:86:MET:O	1:A:90:VAL:HG23	2.20	0.42
3:C:580:PHE:CE2	3:C:620:PRO:HB2	2.55	0.42
1:D:641:LEU:O	1:D:645:VAL:HG23	2.20	0.42
2:E:309:TRP:C	2:E:309:TRP:CD1	2.94	0.42
2:E:438:TRP:HB2	2:E:449:LEU:HD11	2.01	0.42
2:E:663:THR:HB	2:E:666:TRP:CZ2	2.55	0.42
3:F:572:TYR:OH	3:F:604:ARG:NH2	2.52	0.42
1:G:179:ARG:CZ	2:H:711:ILE:HG13	2.50	0.42
1:G:298:GLU:HG3	1:G:488:LYS:NZ	2.35	0.42
2:H:163:LEU:O	2:H:167:LEU:HG	2.20	0.42
3:I:220:VAL:HG12	3:I:223:GLY:H	1.84	0.42
3:I:374:LEU:HD13	3:I:384:LEU:HD13	2.01	0.42
3:I:398:ILE:HD12	3:I:398:ILE:HA	1.95	0.42
3:I:664:ARG:HE	3:I:671:ASP:CG	2.22	0.42
1:J:436:GLU:OE1	2:K:602:ARG:NH2	2.51	0.42
1:J:616:SER:O	1:J:618:THR:HG23	2.20	0.42
2:K:443:SER:OG	2:K:444:SER:N	2.52	0.42
3:L:142:ARG:NE	3:L:486:ASP:HB3	2.35	0.42
1:A:588:SER:OG	1:A:641:LEU:HA	2.19	0.41
3:C:655:VAL:O	3:C:667:VAL:HA	2.20	0.41
1:D:123:THR:OG1	1:D:124:ARG:N	2.52	0.41
1:D:169:ALA:HA	1:D:172:LYS:HE3	2.02	0.41
1:G:337:ALA:O	1:G:341:VAL:HG23	2.20	0.41
2:H:142:ALA:O	2:H:146:THR:OG1	2.28	0.41
3:I:146:ASP:OD1	3:I:146:ASP:N	2.47	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:432:HIS:O	3:I:436:ARG:HG2	2.20	0.41
2:K:283:ALA:O	2:K:287:ARG:HG3	2.19	0.41
2:K:310:ASN:ND2	2:K:407:MET:SD	2.93	0.41
3:L:120:GLU:OE1	3:L:124:ARG:NH2	2.53	0.41
3:L:382:ILE:HD13	3:L:382:ILE:HA	1.90	0.41
3:L:381:LEU:N	3:L:407:GLU:OE2	2.44	0.41
3:L:174:ALA:HA	3:L:726:ILE:HD11	2.02	0.41
2:B:54:LYS:HG3	2:B:68:PRO:HA	2.01	0.41
3:C:107:SER:C	3:C:109:VAL:H	2.22	0.41
3:C:535:MET:O	3:C:537:TRP:CD2	2.73	0.41
1:D:587:GLN:HA	1:D:590:GLN:HG2	2.03	0.41
2:E:437:TRP:NE1	2:E:452:ASN:HB2	2.35	0.41
2:E:598:LEU:HD23	2:E:598:LEU:H	1.85	0.41
3:F:116:LYS:HA	3:F:119:PHE:HD2	1.84	0.41
3:F:753:ARG:HA	3:F:753:ARG:HD2	1.76	0.41
1:G:385:LYS:HG3	1:G:386:ASP:OD1	2.20	0.41
1:G:479:ASP:N	1:G:479:ASP:OD1	2.48	0.41
1:G:491:THR:OG1	1:G:493:GLU:HG2	2.19	0.41
1:G:596:ILE:HG23	1:G:611:PHE:HD2	1.84	0.41
2:H:95:LEU:HG	2:H:425:ASN:HD22	1.85	0.41
3:I:237:GLY:HA3	3:I:240:TRP:CE2	2.55	0.41
3:I:614:GLN:HA	3:I:617:LYS:HB3	2.02	0.41
3:I:55:TYR:HA	3:I:91:VAL:C	2.41	0.41
1:J:113:LYS:HE3	1:J:113:LYS:HB3	1.83	0.41
2:K:519:GLU:HB3	2:K:664:HIS:CD2	2.55	0.41
2:K:58:ASN:OD1	2:K:60:GLU:N	2.51	0.41
2:K:49:TYR:CE1	2:K:79:PRO:HG2	2.56	0.41
1:A:326:HIS:O	1:A:326:HIS:ND1	2.53	0.41
1:A:180:GLN:NE2	3:C:174:ALA:H	2.19	0.41
1:D:354:ILE:HA	1:D:355:PRO:HD3	1.71	0.41
2:E:550:LEU:HA	2:E:550:LEU:HD23	1.94	0.41
2:E:735:ILE:HA	2:E:735:ILE:HD12	1.94	0.41
1:G:219:LEU:H	1:G:219:LEU:HG	1.70	0.41
1:G:420:SER:HA	1:G:490:ARG:O	2.20	0.41
1:G:568:ASN:OD1	1:G:569:GLY:N	2.45	0.41
2:H:188:LYS:HB2	2:H:188:LYS:HE3	1.93	0.41
2:H:420:GLY:HA3	2:H:442:GLN:HG2	2.00	0.41
2:H:497:TYR:HA	2:H:500:GLY:O	2.20	0.41
1:J:432:VAL:HG22	1:J:436:GLU:OE1	2.20	0.41
2:K:318:PHE:HA	2:K:321:MET:HG2	2.02	0.41
1:A:612:PHE:CE1	1:A:633:ILE:HG21	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:73:LYS:HE3	1:A:112:TYR:HE2	1.85	0.41
2:B:99:HIS:HA	2:B:100:PRO:HD3	1.86	0.41
2:B:382:ASN:ND2	2:B:385:THR:OG1	2.45	0.41
2:B:602:ARG:O	3:C:125:LEU:HD21	2.20	0.41
3:C:333:THR:HB	3:C:362:GLU:O	2.20	0.41
3:C:176:ILE:HG22	3:C:693:GLY:HA3	2.02	0.41
1:D:434:PRO:HG2	3:F:130:PHE:CD1	2.55	0.41
2:E:523:MET:HA	2:E:551:PHE:HZ	1.85	0.41
3:F:407:GLU:O	3:F:410:MET:HG3	2.21	0.41
3:F:454:ILE:HG12	3:F:472:GLU:C	2.40	0.41
2:H:252:VAL:HG23	2:H:412:PHE:HE1	1.85	0.41
2:H:318:PHE:HA	2:H:321:MET:HG2	2.03	0.41
2:H:414:MET:O	2:H:418:VAL:HG23	2.21	0.41
3:I:260:ILE:O	3:I:264:ARG:HG3	2.20	0.41
3:I:264:ARG:HE	3:I:305:GLU:CD	2.24	0.41
3:I:6:GLU:O	3:I:10:LEU:HB2	2.19	0.41
1:J:309:LYS:HG2	1:J:309:LYS:H	1.61	0.41
2:K:485:ASN:OD1	2:K:485:ASN:N	2.54	0.41
3:L:421:VAL:HB	3:L:426:GLN:N	2.35	0.41
3:L:325:PHE:HZ	3:L:431:MET:HB3	1.86	0.41
1:A:504:ILE:HA	1:A:521:VAL:O	2.21	0.41
1:A:74:HIS:C	1:A:76:PHE:N	2.74	0.41
2:B:579:LEU:HA	2:B:579:LEU:HD23	1.78	0.41
3:C:260:ILE:O	3:C:264:ARG:HG3	2.20	0.41
3:C:358:GLU:HG2	3:C:359:GLY:H	1.86	0.41
1:D:125:ARG:HH22	1:D:130:TYR:HD1	1.67	0.41
2:E:146:THR:HG22	2:E:150:PHE:CE2	2.56	0.41
3:F:39:GLN:H	3:F:39:GLN:HG2	1.64	0.41
3:F:408:ASP:O	3:F:412:LYS:HG2	2.20	0.41
3:F:453:PRO:HA	3:F:473:MET:HG2	2.03	0.41
1:G:586:LEU:HD21	2:H:547:ALA:N	2.35	0.41
1:J:328:LYS:HA	1:J:328:LYS:HD3	1.88	0.41
1:J:611:PHE:CE1	1:J:619:TRP:HZ2	2.39	0.41
1:J:614:ASN:OD1	1:J:617:GLU:N	2.52	0.41
3:L:144:ARG:HE	3:L:489:SER:HB2	1.85	0.41
1:A:278:GLN:HG2	1:A:280:SER:H	1.85	0.41
1:A:588:SER:O	1:A:591:GLN:HG2	2.21	0.41
2:B:52:LYS:HD3	2:B:52:LYS:HA	1.76	0.41
3:C:535:MET:CG	3:C:536:MET:H	2.31	0.41
1:D:548:MET:O	1:D:558:SER:HA	2.20	0.41
2:E:751:GLU:O	2:E:754:ARG:HG2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:595:PHE:CE2	3:F:633:PHE:HB2	2.55	0.41
2:H:155:LEU:HD12	2:H:155:LEU:H	1.85	0.41
2:H:420:GLY:O	2:H:423:ILE:HG22	2.20	0.41
2:H:578:LYS:HE3	3:I:101:ARG:HH12	1.84	0.41
3:I:306:GLN:O	3:I:310:ILE:HG13	2.21	0.41
3:I:584:ILE:HG13	3:I:585:PRO:HD2	2.03	0.41
1:J:577:TRP:HZ2	1:J:648:SER:HA	1.85	0.41
1:J:588:SER:O	1:J:591:GLN:HG2	2.20	0.41
1:J:612:PHE:CE1	1:J:633:ILE:HG21	2.51	0.41
2:K:424:LEU:HD11	2:K:442:GLN:HB2	2.02	0.41
2:K:663:THR:HB	2:K:666:TRP:HZ2	1.85	0.41
2:K:698:LYS:HB2	2:K:698:LYS:HE2	1.67	0.41
3:L:452:GLU:CD	3:L:476:ARG:HA	2.41	0.41
1:A:262:LYS:HB3	1:A:672:LEU:HD11	2.02	0.41
2:B:415:LEU:HD12	2:B:418:VAL:HB	2.01	0.41
2:B:623:ARG:NE	3:C:103:GLY:H	2.19	0.41
3:C:471:THR:OG1	3:C:472:GLU:OE1	2.21	0.41
2:B:708:PRO:HB3	3:C:728:GLN:HE21	1.85	0.41
1:D:335:LEU:HD12	1:D:336:LEU:HD12	2.03	0.41
1:D:293:GLU:H	1:D:497:LYS:HG3	1.85	0.41
1:D:67:ASP:HA	1:D:68:PRO:HD3	1.94	0.41
2:E:697:GLU:HA	2:E:703:SER:OG	2.20	0.41
3:F:658:TYR:CE1	3:F:663:LYS:HA	2.55	0.41
1:G:540:TYR:CE1	1:G:566:ARG:HB3	2.55	0.41
3:I:323:PHE:HB2	3:I:330:PHE:HB2	2.03	0.41
3:I:482:LYS:HG2	3:I:483:MET:HE2	2.02	0.41
1:J:12:MET:O	1:J:16:LEU:HG	2.21	0.41
2:K:4:ASN:HB3	2:K:7:LEU:HG	2.03	0.41
3:L:230:GLU:HG3	3:L:231:VAL:HG13	2.03	0.41
3:L:399:ILE:HD13	3:L:399:ILE:HA	1.84	0.41
3:L:39:GLN:H	3:L:39:GLN:HG2	1.58	0.41
3:L:505:ARG:HD3	3:L:509:GLY:HA2	2.02	0.41
1:A:149:PRO:HD2	1:A:153:GLU:O	2.21	0.41
1:A:459:ILE:O	1:A:463:VAL:HG23	2.21	0.41
1:A:595:MET:SD	2:B:17:ALA:HB2	2.61	0.41
2:B:271:LEU:N	2:B:272:PRO:HD2	2.36	0.41
2:B:36:THR:HG21	2:B:354:GLY:N	2.35	0.41
3:C:28:ILE:HA	3:C:31:ILE:HG22	2.03	0.41
1:D:326:HIS:CE1	1:D:539:LYS:HA	2.55	0.41
1:D:363:THR:HB	1:D:365:GLN:OE1	2.21	0.41
1:D:665:LEU:O	1:D:669:VAL:HG23	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:595:MET:CG	2:E:17:ALA:HB2	2.51	0.41
2:E:47:HIS:CE1	2:E:55:TRP:HH2	2.39	0.41
1:G:641:LEU:O	1:G:645:VAL:HG23	2.19	0.41
2:H:122:LEU:HA	2:H:122:LEU:HD12	1.95	0.41
2:H:68:PRO:HD2	2:H:314:ASN:HD21	1.85	0.41
1:J:33:ASN:OD1	1:J:193:GLN:HG2	2.20	0.41
2:K:660:VAL:O	2:K:662:THR:HG23	2.20	0.41
3:L:368:ARG:NH1	3:L:520:GLU:OE1	2.54	0.41
3:L:635:SER:HB2	3:L:646:ARG:HH11	1.84	0.41
2:B:309:TRP:CD1	2:B:309:TRP:C	2.94	0.41
1:A:253:VAL:O	2:B:468:ARG:HD3	2.20	0.41
2:B:519:GLU:OE1	2:B:664:HIS:NE2	2.52	0.41
3:C:39:GLN:HG2	3:C:39:GLN:H	1.59	0.41
3:C:634:SER:O	3:C:649:VAL:HG13	2.20	0.41
1:D:392:GLN:HG2	1:D:393:TYR:H	1.86	0.41
2:E:660:VAL:O	2:E:662:THR:HG23	2.21	0.41
1:G:425:LEU:HA	1:G:425:LEU:HD12	1.92	0.41
1:G:484:PRO:HB2	1:G:486:ILE:HG13	2.02	0.41
2:H:261:SER:O	2:H:265:LYS:HE2	2.21	0.41
2:H:283:ALA:O	2:H:286:VAL:HB	2.20	0.41
2:H:599:TYR:HE1	2:H:608:GLU:HA	1.86	0.41
1:J:459:ILE:O	1:J:463:VAL:HG23	2.20	0.41
1:J:483:ILE:HD11	1:J:506:LYS:HB2	2.03	0.41
1:J:266:ARG:HG3	1:J:687:TYR:CE2	2.55	0.41
3:L:63:ILE:HG12	3:L:63:ILE:H	1.66	0.41
1:A:163:LEU:HD22	1:A:164:ASP:H	1.86	0.41
1:A:443:ARG:NH1	2:B:549:GLN:HE22	2.19	0.41
1:A:318:LYS:HB2	1:A:546:GLY:HA2	2.03	0.41
2:B:626:ASN:OD1	2:B:628:LEU:HB2	2.21	0.41
3:C:371:THR:HG21	3:C:487:GLU:HG3	2.01	0.41
3:C:376:LYS:HA	3:C:380:ARG:O	2.21	0.41
1:D:274:PRO:HA	1:D:275:PRO:HD3	1.96	0.41
1:D:560:PRO:HB2	1:D:562:PHE:CE1	2.56	0.41
3:F:286:SER:HB3	3:F:533:SER:HB3	2.02	0.41
3:F:498:ILE:HD11	3:F:502:LEU:HA	2.03	0.41
3:F:619:LEU:O	3:F:622:THR:HG23	2.21	0.41
1:G:318:LYS:HG2	1:G:319:GLU:H	1.85	0.41
2:H:315:PRO:HA	2:H:318:PHE:CD2	2.52	0.41
1:G:218:SER:HA	2:H:345:SER:OG	2.21	0.41
1:J:623:GLU:HA	1:J:627:GLY:O	2.21	0.41
1:A:617:GLU:HB3	1:A:619:TRP:CZ3	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:392:GLN:HG2	1:D:393:TYR:N	2.36	0.41
2:E:225:ASN:OD1	2:E:226:THR:N	2.37	0.41
2:E:318:PHE:HA	2:E:321:MET:HG2	2.02	0.41
3:F:170:ASN:OD1	3:F:709:SER:OG	2.37	0.41
3:F:1:MET:HA	3:F:4:ILE:HG22	2.02	0.41
3:I:135:PHE:CE2	3:I:240:TRP:HB3	2.56	0.41
3:I:264:ARG:HH21	3:I:305:GLU:CG	2.34	0.41
3:I:332:ARG:HA	3:I:363:PHE:HD1	1.86	0.41
1:J:592:ILE:O	1:J:596:ILE:HG13	2.20	0.41
1:J:276:CYS:HB2	1:J:698:PRO:HG3	2.01	0.41
2:K:290:MET:SD	2:K:299:SER:HB3	2.61	0.41
2:K:339:ILE:O	2:K:343:MET:HG3	2.21	0.41
3:L:152:ALA:N	3:L:252:ASN:OD1	2.53	0.41
1:A:116:ARG:HD3	1:A:144:HIS:HB2	2.02	0.40
1:A:168:ARG:HG2	1:A:172:LYS:HE3	2.01	0.40
2:B:599:TYR:OH	2:B:608:GLU:N	2.55	0.40
3:C:358:GLU:HG2	3:C:359:GLY:N	2.36	0.40
1:D:365:GLN:H	1:D:365:GLN:CD	2.24	0.40
1:D:476:ALA:HB3	1:D:506:LYS:HE2	2.02	0.40
2:E:10:LEU:HA	2:E:10:LEU:HD23	1.94	0.40
2:E:218:LEU:O	2:E:222:LEU:HG	2.20	0.40
1:G:443:ARG:HG3	1:G:444:ASN:N	2.35	0.40
1:G:545:ILE:HA	1:G:545:ILE:HD12	1.82	0.40
1:G:77:GLU:OE1	1:G:112:TYR:OH	2.21	0.40
2:H:707:ARG:HA	2:H:708:PRO:HD3	1.94	0.40
1:G:7:GLN:HA	3:I:299:ARG:CZ	2.51	0.40
3:I:384:LEU:HD21	3:I:398:ILE:HD11	2.02	0.40
1:J:438:ILE:HA	1:J:441:MET:HG2	2.03	0.40
1:J:52:HIS:O	1:J:75:ARG:HB3	2.21	0.40
1:J:545:ILE:HD12	1:J:545:ILE:HA	1.87	0.40
1:J:623:GLU:O	2:K:2:ASP:HB2	2.22	0.40
2:K:305:ASP:HA	2:K:445:ASP:O	2.20	0.40
3:L:28:ILE:HA	3:L:31:ILE:HG22	2.03	0.40
1:A:188:TRP:CD1	1:A:191:PHE:HB2	2.56	0.40
1:A:33:ASN:ND2	1:A:189:ASP:OD1	2.54	0.40
1:A:205:PHE:HE2	2:B:339:ILE:HD11	1.85	0.40
3:C:385:ILE:HG13	3:C:479:ARG:HB2	2.03	0.40
1:D:258:GLU:HA	1:D:259:PRO:HD3	1.95	0.40
2:E:222:LEU:HB3	2:E:347:LYS:HA	2.03	0.40
2:E:692:CYS:SG	3:F:10:LEU:HD21	2.61	0.40
3:F:364:THR:HG22	3:F:373:ILE:HD12	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:576:LEU:HD12	3:F:97:THR:HG21	2.03	0.40
1:G:106:LEU:HD23	1:G:107:PRO:HD2	2.02	0.40
1:G:392:GLN:HG2	1:G:393:TYR:N	2.37	0.40
1:G:338:TRP:HE1	1:G:545:ILE:HD11	1.85	0.40
2:H:665:SER:C	2:H:666:TRP:HD1	2.24	0.40
2:H:750:ILE:HD13	3:I:4:ILE:HD11	2.03	0.40
3:I:281:LEU:HA	3:I:281:LEU:HD23	1.91	0.40
3:I:535:MET:O	3:I:537:TRP:CD2	2.75	0.40
1:J:361:LYS:HE2	1:J:361:LYS:HB3	1.92	0.40
2:K:666:TRP:O	3:L:50:MET:HE1	2.21	0.40
3:L:16:THR:HA	3:L:19:ILE:HG22	2.04	0.40
3:L:225:SER:OG	3:L:226:SER:N	2.54	0.40
3:C:499:ASP:HB3	3:C:505:ARG:NH1	2.29	0.40
1:D:385:LYS:HG3	1:D:386:ASP:OD1	2.21	0.40
2:E:52:LYS:HA	2:E:52:LYS:HD3	1.81	0.40
2:E:620:TYR:CZ	2:E:624:LEU:HD12	2.56	0.40
2:E:626:ASN:HB3	3:F:99:TRP:CZ2	2.57	0.40
2:E:626:ASN:ND2	3:F:106:THR:OG1	2.54	0.40
1:G:179:ARG:HG2	1:G:188:TRP:CZ3	2.56	0.40
1:G:577:TRP:CZ2	1:G:648:SER:HA	2.56	0.40
2:H:297:GLU:OE2	2:H:454:PRO:HB3	2.21	0.40
3:I:112:PRO:HB3	3:I:119:PHE:CD2	2.56	0.40
3:I:333:THR:OG1	3:I:364:THR:HG23	2.22	0.40
3:I:384:LEU:HB3	3:I:477:GLY:O	2.21	0.40
3:I:71:ASN:OD1	3:I:74:GLY:N	2.54	0.40
1:J:492:LYS:HA	1:J:492:LYS:HD2	1.92	0.40
1:J:583:ARG:HH12	2:K:509:LEU:HG	1.87	0.40
1:J:643:LYS:O	1:J:647:ASN:ND2	2.55	0.40
1:J:221:PRO:HG3	2:K:67:ASN:HB3	2.02	0.40
2:K:697:GLU:HA	2:K:703:SER:OG	2.21	0.40
3:L:396:GLU:O	3:L:400:VAL:HG12	2.21	0.40
3:L:429:ASN:OD1	3:L:429:ASN:N	2.53	0.40
3:L:571:LEU:HD21	3:L:619:LEU:HD21	2.02	0.40
1:A:198:GLU:HG2	1:A:200:THR:HG22	2.04	0.40
1:A:385:LYS:HG3	1:A:386:ASP:OD1	2.21	0.40
2:B:565:ASP:HB2	2:B:580:TRP:CZ2	2.55	0.40
2:B:689:TYR:HD1	3:C:31:ILE:HD11	1.85	0.40
2:B:687:GLN:O	2:B:691:LYS:HD2	2.21	0.40
3:C:146:ASP:OD1	3:C:146:ASP:N	2.54	0.40
1:D:10:ASN:OD1	1:D:13:ILE:N	2.39	0.40
1:D:261:LEU:HA	1:D:261:LEU:HD12	1.95	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:290:LEU:O	1:D:292:ILE:HG13	2.22	0.40
1:D:54:ILE:CG1	1:D:75:ARG:HD3	2.51	0.40
1:D:407:ILE:HG23	1:D:702:LEU:HD22	2.03	0.40
2:E:314:ASN:OD1	2:E:315:PRO:HD2	2.22	0.40
2:E:22:PHE:CE2	2:E:504:ASN:HB3	2.56	0.40
2:E:698:LYS:HB2	2:E:698:LYS:HE2	1.85	0.40
1:G:529:ASP:N	1:G:529:ASP:OD1	2.54	0.40
2:H:66:LEU:HA	2:H:66:LEU:HD23	1.95	0.40
1:J:425:LEU:HA	1:J:425:LEU:HD12	1.89	0.40
1:J:289:LYS:HB3	1:J:499:ASN:OD1	2.21	0.40
1:J:548:MET:O	1:J:558:SER:HA	2.21	0.40
1:J:621:ILE:O	2:K:4:ASN:N	2.31	0.40
3:L:227:VAL:O	3:L:231:VAL:HG22	2.20	0.40
3:L:333:THR:OG1	3:L:364:THR:HG23	2.20	0.40
1:A:168:ARG:O	1:A:172:LYS:HG3	2.22	0.40
1:A:48:TYR:HD1	1:A:48:TYR:O	2.05	0.40
3:C:584:ILE:HD11	3:C:592:TYR:CD2	2.53	0.40
1:D:381:PHE:HA	1:D:384:CYS:SG	2.61	0.40
1:D:523:MET:HB3	1:D:563:LEU:HD11	2.02	0.40
2:E:374:ALA:O	2:E:393:ARG:NH2	2.55	0.40
2:E:485:ASN:OD1	2:E:485:ASN:N	2.55	0.40
3:F:339:LYS:HG3	3:F:340:LYS:H	1.86	0.40
3:F:559:THR:O	3:F:562:ILE:CD1	2.69	0.40
1:G:524:GLU:O	1:G:563:LEU:HD12	2.21	0.40
2:H:339:ILE:O	2:H:343:MET:HG3	2.20	0.40
2:K:68:PRO:HD2	2:K:314:ASN:ND2	2.37	0.40
3:L:744:LEU:C	3:L:746:ASP:H	2.25	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:415:ARG:NH2	3:I:448:ASN:OD1[4_545]	2.19	0.01

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	714/716 (100%)	654 (92%)	60 (8%)	0	100	100
1	D	714/716 (100%)	652 (91%)	62 (9%)	0	100	100
1	G	714/716 (100%)	648 (91%)	66 (9%)	0	100	100
1	J	706/716 (99%)	647 (92%)	57 (8%)	2 (0%)	41	74
2	B	671/757 (89%)	611 (91%)	60 (9%)	0	100	100
2	E	647/757 (86%)	594 (92%)	53 (8%)	0	100	100
2	H	659/757 (87%)	599 (91%)	59 (9%)	1 (0%)	47	79
2	K	648/757 (86%)	600 (93%)	48 (7%)	0	100	100
3	C	719/765 (94%)	649 (90%)	69 (10%)	1 (0%)	51	83
3	F	723/765 (94%)	645 (89%)	77 (11%)	1 (0%)	51	83
3	I	712/765 (93%)	643 (90%)	69 (10%)	0	100	100
3	L	722/765 (94%)	652 (90%)	68 (9%)	2 (0%)	41	74
All	All	8349/8952 (93%)	7594 (91%)	748 (9%)	7 (0%)	51	83

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	536	MET
3	F	535	MET
2	H	429	LYS
3	L	535	MET
3	L	745	THR
1	J	434	PRO
1	J	435	ILE

5.3.2 Protein sidechains [i](#)

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	640/640 (100%)	625 (98%)	15 (2%)	50	75
1	D	640/640 (100%)	622 (97%)	18 (3%)	43	71
1	G	640/640 (100%)	626 (98%)	14 (2%)	52	76
1	J	635/640 (99%)	620 (98%)	15 (2%)	49	74
2	B	605/668 (91%)	593 (98%)	12 (2%)	55	78
2	E	587/668 (88%)	577 (98%)	10 (2%)	60	81
2	H	597/668 (89%)	587 (98%)	10 (2%)	60	81
2	K	585/668 (88%)	574 (98%)	11 (2%)	57	79
3	C	643/674 (95%)	637 (99%)	6 (1%)	78	89
3	F	647/674 (96%)	637 (98%)	10 (2%)	65	83
3	I	639/674 (95%)	630 (99%)	9 (1%)	67	84
3	L	646/674 (96%)	632 (98%)	14 (2%)	52	76
All	All	7504/7928 (95%)	7360 (98%)	144 (2%)	57	79

All (144) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	PHE
1	A	35	PHE
1	A	48	TYR
1	A	57	ARG
1	A	74	HIS
1	A	130	TYR
1	A	146	HIS
1	A	163	LEU
1	A	282	PHE
1	A	362	LYS
1	A	426	ASP
1	A	529	ASP
1	A	537	TRP
1	A	549	LEU
1	A	611	PHE
2	B	67	ASN
2	B	116	GLN
2	B	153	ASN
2	B	175	ASP
2	B	184	HIS
2	B	211	ARG
2	B	309	TRP

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Mol	Chain	Res	Type
2	B	557	TYR
2	B	579	LEU
2	B	638	GLU
2	B	670	ARG
2	B	699	PHE
3	C	38	ARG
3	C	110	HIS
3	C	256	ASP
3	C	306	GLN
3	C	323	PHE
3	C	535	MET
1	D	4	PHE
1	D	12	MET
1	D	35	PHE
1	D	48	TYR
1	D	57	ARG
1	D	74	HIS
1	D	119	GLU
1	D	130	TYR
1	D	163	LEU
1	D	219	LEU
1	D	350	ASN
1	D	362	LYS
1	D	426	ASP
1	D	427	GLU
1	D	443	ARG
1	D	479	ASP
1	D	549	LEU
1	D	611	PHE
2	E	67	ASN
2	E	153	ASN
2	E	175	ASP
2	E	309	TRP
2	E	310	ASN
2	E	509	LEU
2	E	536	ASN
2	E	557	TYR
2	E	579	LEU
2	E	636	GLU
3	F	38	ARG
3	F	70	ARG
3	F	111	TYR

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Mol	Chain	Res	Type
3	F	134	HIS
3	F	205	TYR
3	F	306	GLN
3	F	323	PHE
3	F	500	ARG
3	F	505	ARG
3	F	721	LYS
1	G	4	PHE
1	G	35	PHE
1	G	48	TYR
1	G	57	ARG
1	G	74	HIS
1	G	130	TYR
1	G	163	LEU
1	G	362	LYS
1	G	426	ASP
1	G	427	GLU
1	G	443	ARG
1	G	529	ASP
1	G	549	LEU
1	G	611	PHE
2	H	41	ASP
2	H	67	ASN
2	H	175	ASP
2	H	276	ASN
2	H	309	TRP
2	H	446	ASP
2	H	507	MET
2	H	509	LEU
2	H	557	TYR
2	H	699	PHE
3	I	38	ARG
3	I	46	ARG
3	I	70	ARG
3	I	111	TYR
3	I	134	HIS
3	I	196	CYS
3	I	500	ARG
3	I	535	MET
3	I	657	ASN
1	J	4	PHE
1	J	7	GLN

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Mol	Chain	Res	Type
1	J	27	ASP
1	J	35	PHE
1	J	48	TYR
1	J	57	ARG
1	J	74	HIS
1	J	130	TYR
1	J	350	ASN
1	J	362	LYS
1	J	426	ASP
1	J	427	GLU
1	J	549	LEU
1	J	603	LYS
1	J	611	PHE
2	K	67	ASN
2	K	153	ASN
2	K	175	ASP
2	K	276	ASN
2	K	309	TRP
2	K	446	ASP
2	K	509	LEU
2	K	557	TYR
2	K	579	LEU
2	K	582	GLN
2	K	699	PHE
3	L	38	ARG
3	L	46	ARG
3	L	100	ASN
3	L	134	HIS
3	L	195	ASP
3	L	196	CYS
3	L	202	MET
3	L	306	GLN
3	L	323	PHE
3	L	458	MET
3	L	508	ARG
3	L	535	MET
3	L	702	LYS
3	L	738	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	146	HIS
1	A	193	GLN
2	B	116	GLN
2	B	367	GLN
2	B	605	HIS
2	B	626	ASN
2	B	671	ASN
3	C	110	HIS
3	C	138	GLN
3	C	257	GLN
3	C	551	GLN
3	C	614	GLN
1	D	193	GLN
1	D	587	GLN
1	D	591	GLN
2	E	312	ASN
2	E	314	ASN
2	E	605	HIS
1	G	144	HIS
1	G	146	HIS
1	G	510	HIS
1	G	587	GLN
2	H	312	ASN
2	H	425	ASN
2	H	605	HIS
3	I	110	HIS
3	I	252	ASN
3	I	728	GLN
1	J	7	GLN
2	K	312	ASN
3	L	406	GLN

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](#)

There are no ligands in this entry.

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	716/716 (100%)	-0.02	4 (0%) 89 81	39, 83, 142, 203	0
1	D	716/716 (100%)	0.19	19 (2%) 54 38	56, 106, 163, 212	0
1	G	716/716 (100%)	0.06	5 (0%) 87 79	42, 82, 147, 205	0
1	J	710/716 (99%)	0.08	13 (1%) 68 53	59, 101, 145, 200	0
2	B	685/757 (90%)	0.15	12 (1%) 68 53	49, 85, 137, 215	0
2	E	661/757 (87%)	0.21	12 (1%) 68 53	64, 108, 152, 240	0
2	H	673/757 (88%)	0.11	7 (1%) 82 71	39, 88, 138, 185	0
2	K	662/757 (87%)	0.18	5 (0%) 86 76	44, 98, 142, 202	0
3	C	727/765 (95%)	0.14	18 (2%) 57 41	55, 103, 163, 227	0
3	F	731/765 (95%)	0.31	26 (3%) 42 29	64, 119, 176, 210	0
3	I	722/765 (94%)	0.16	15 (2%) 63 48	46, 99, 151, 179	0
3	L	730/765 (95%)	0.16	11 (1%) 73 60	55, 100, 160, 232	0
All	All	8449/8952 (94%)	0.14	147 (1%) 70 56	39, 97, 155, 240	0

All (147) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	665	SER	7.8
3	F	717	ALA	7.3
3	F	510	ASN	6.0
3	I	456	ASN	5.2
1	D	68	PRO	5.2
3	L	483	MET	4.4
1	A	391	LYS	4.3
3	L	522	GLN	4.2
2	K	267	GLU	4.0
2	E	398	ASP	4.0
3	L	250	VAL	4.0

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Mol	Chain	Res	Type	RSRZ
1	D	244	GLY	3.7
3	F	456	ASN	3.7
3	L	755	ARG	3.7
3	I	343	GLU	3.5
2	H	665	SER	3.5
1	G	67	ASP	3.5
1	D	67	ASP	3.4
3	F	751	THR	3.4
2	B	53	GLY	3.3
1	D	715	LEU	3.3
1	G	126	GLU	3.3
3	C	432	HIS	3.2
3	F	327	GLY	3.2
3	I	717	ALA	3.2
3	C	467	MET	3.2
1	D	195	GLU	3.1
3	F	440	LYS	3.0
3	L	756	MET	3.0
3	C	451	ILE	3.0
3	L	489	SER	3.0
1	D	599	GLU	3.0
3	I	485	VAL	2.9
3	F	489	SER	2.9
3	I	578	GLU	2.9
3	F	522	GLN	2.9
3	C	426	GLN	2.9
3	I	236	GLN	2.9
3	F	396	GLU	2.8
3	F	754	ILE	2.8
2	B	212	LEU	2.8
2	B	378	LEU	2.8
3	F	37	GLY	2.7
1	D	610	GLU	2.7
3	F	358	GLU	2.7
1	J	126	GLU	2.7
3	C	442	ALA	2.7
3	C	271	THR	2.6
3	F	138	GLN	2.6
1	J	695	ILE	2.6
1	D	69	ASN	2.6
1	J	610	GLU	2.6
3	C	18	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
1	J	67	ASP	2.6
3	F	486	ASP	2.6
1	D	716	ARG	2.6
3	C	275	ASP	2.6
1	D	542	VAL	2.6
3	I	39	GLN	2.5
1	J	214	LEU	2.5
3	F	65	GLU	2.5
2	B	75	ASP	2.5
3	F	332	ARG	2.5
1	D	695	ILE	2.5
2	H	725	ASP	2.5
3	F	756	MET	2.5
2	B	210	GLN	2.5
2	E	634	HIS	2.5
3	F	693	GLY	2.5
3	F	252	ASN	2.5
2	B	501	PHE	2.5
2	E	584	ARG	2.4
2	K	261	SER	2.4
2	K	403	LEU	2.4
3	L	717	ALA	2.4
3	C	521	THR	2.4
1	G	553	ALA	2.4
3	C	191	GLU	2.4
3	I	341	GLU	2.4
3	F	403	VAL	2.4
2	E	8	LEU	2.4
1	D	291	SER	2.4
3	C	39	GLN	2.3
3	F	359	GLY	2.3
1	A	216	ASP	2.3
2	B	440	GLY	2.3
3	F	142	ARG	2.3
1	J	58	GLY	2.3
3	C	567	ASP	2.3
1	D	243	GLU	2.3
1	D	349	GLU	2.3
2	B	165	ASP	2.3
1	J	216	ASP	2.3
1	D	409	SER	2.3
2	E	378	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	G	626	LYS	2.3
3	C	509	GLY	2.3
3	I	436	ARG	2.3
3	I	486	ASP	2.3
2	B	173	SER	2.2
2	E	410	GLY	2.2
2	B	375	ASN	2.2
2	K	717	ALA	2.2
2	H	294	GLN	2.2
2	E	658	ASP	2.2
1	D	237	GLU	2.2
3	I	521	THR	2.2
1	J	149	PRO	2.2
3	L	533	SER	2.2
1	D	398	PRO	2.2
1	D	660	ALA	2.2
3	L	439	GLN	2.2
1	D	620	PRO	2.2
2	H	53	GLY	2.2
1	J	213	ARG	2.1
2	H	494	SER	2.1
1	J	23	GLU	2.1
3	L	39	GLN	2.1
3	C	513	LEU	2.1
3	I	671	ASP	2.1
2	H	625	CYS	2.1
3	C	365	MET	2.1
1	A	81	GLY	2.1
3	I	108	THR	2.1
1	J	299	GLY	2.1
3	F	467	MET	2.1
2	B	169	ASP	2.1
2	K	725	ASP	2.1
3	C	393	SER	2.1
3	I	569	THR	2.1
3	F	753	ARG	2.1
2	B	115	GLN	2.1
3	C	531	TYR	2.1
3	L	324	SER	2.1
3	F	105	THR	2.1
2	E	118	ARG	2.1
3	C	506	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
2	H	306	ASN	2.1
1	A	83	ASP	2.1
3	F	333	THR	2.1
2	E	638	GLU	2.1
1	J	140	SER	2.0
2	E	633	SER	2.0
1	J	478	ASP	2.0
2	E	450	ILE	2.0
1	G	596	ILE	2.0
3	I	487	GLU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.