Full wwPDB X-ray Structure Validation Report (i)

Dec 17, 2023 – 09:47 pm GMT

PDB ID	:	4B8C
Title	:	nuclease module of the yeast Ccr4-Not complex
Authors	:	Basquin, J.; Conti, E.
Deposited on	:	2012-08-26
Resolution	:	3.41 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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

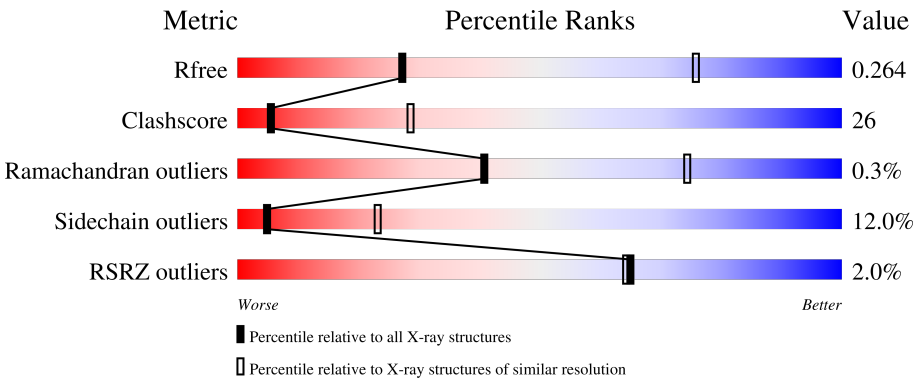
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.41 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	1486 (3.50-3.34)
Clashscore	141614	1572 (3.50-3.34)
Ramachandran outliers	138981	1534 (3.50-3.34)
Sidechain outliers	138945	1535 (3.50-3.34)
RSRZ outliers	127900	1395 (3.50-3.34)

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 of 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 <=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	288	60% 27% 6% 7%
1	C	288	% 59% 28% 6% 7%
1	E	288	61% 27% • 7%
1	F	288	64% 24% 5% 7%
2	B	249	% 65% 27% • 6%

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Mol	Chain	Length	Quality of chain
2	G	249	% 61% 30% • 6%
2	H	249	2% 61% 31% • 6%
2	I	249	2% 62% 29% • 6%
3	D	727	2% 16% 23% • 56%
3	J	727	% 11% 14% • 71%
3	K	727	3% 18% 21% 5% 56%
3	L	727	11% 14% • 71%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 24298 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 POLY(A) RIBONUCLEASE POP2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	267	2170	1409	346	404	11	0	0	0
1	C	267	2174	1412	347	404	11	0	0	0
1	E	267	2174	1411	347	405	11	0	0	0
1	F	267	2170	1409	346	404	11	0	0	0

- Molecule 2 is a protein called GENERAL NEGATIVE REGULATOR OF TRANSCRIPTION SUBUNIT 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	233	1869	1221	309	333	6	0	0	0
2	G	233	1869	1221	309	333	6	0	0	0
2	H	233	1869	1221	309	333	6	0	0	0
2	I	233	1869	1221	309	333	6	0	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	752	ARG	-	expression tag	UNP P25655
B	753	SER	-	expression tag	UNP P25655
B	754	MET	-	expression tag	UNP P25655
G	752	ARG	-	expression tag	UNP P25655
G	753	SER	-	expression tag	UNP P25655
G	754	MET	-	expression tag	UNP P25655
H	752	ARG	-	expression tag	UNP P25655
H	753	SER	-	expression tag	UNP P25655

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Chain	Residue	Modelled	Actual	Comment	Reference
H	754	MET	-	expression tag	UNP P25655
I	752	ARG	-	expression tag	UNP P25655
I	753	SER	-	expression tag	UNP P25655
I	754	MET	-	expression tag	UNP P25655

- Molecule 3 is a protein called GLUCOSE-REPRESSIBLE ALCOHOL DEHYDROGENASE TRANSCRIPTIONAL EFFECTOR.

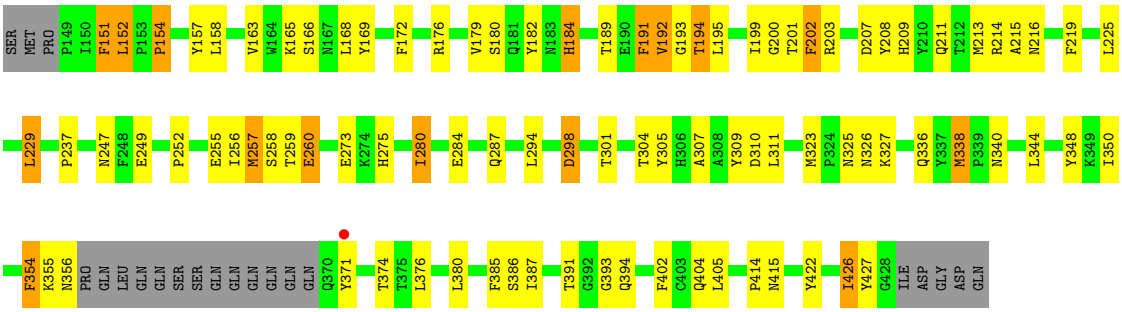
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	D	318	2456	1599	387	459	11	0	0	0
			Total	C	N	O	S			
3	J	210	1604	1034	266	298	6	0	0	0
			Total	C	N	O	S			
3	K	318	2470	1608	392	459	11	0	0	0
			Total	C	N	O	S			
3	L	210	1604	1034	266	298	6	0	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

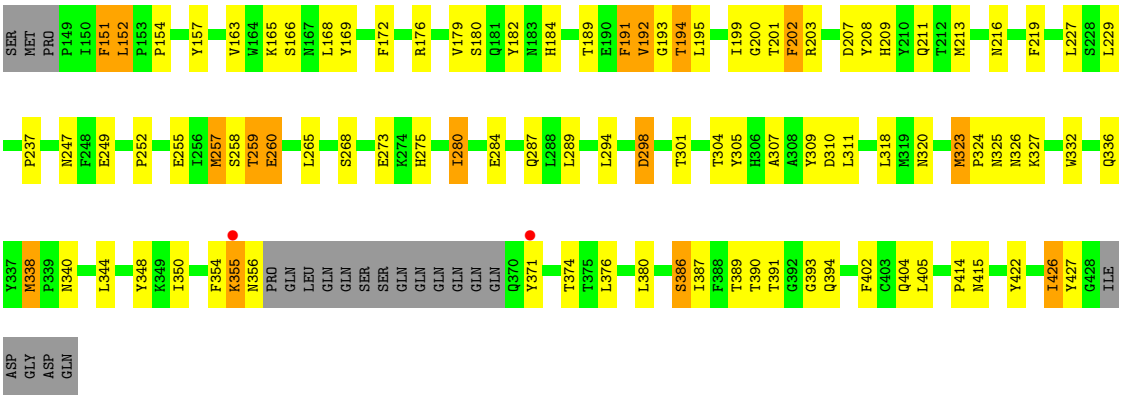
• Molecule 1: POLY(A) RIBONUCLEASE POP2

Chain A: 60% 27% 6% 7%



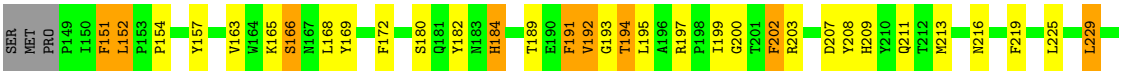
• Molecule 1: POLY(A) RIBONUCLEASE POP2

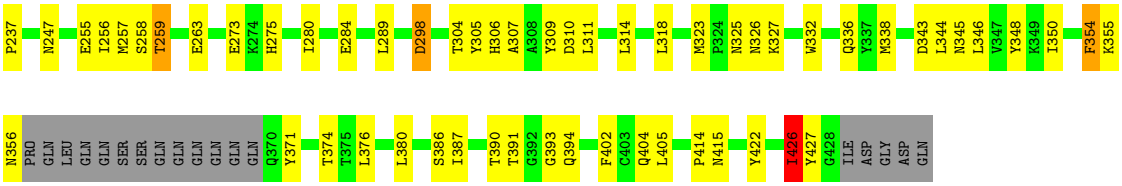
Chain C: % 59% 28% 6% 7%



• Molecule 1: POLY(A) RIBONUCLEASE POP2

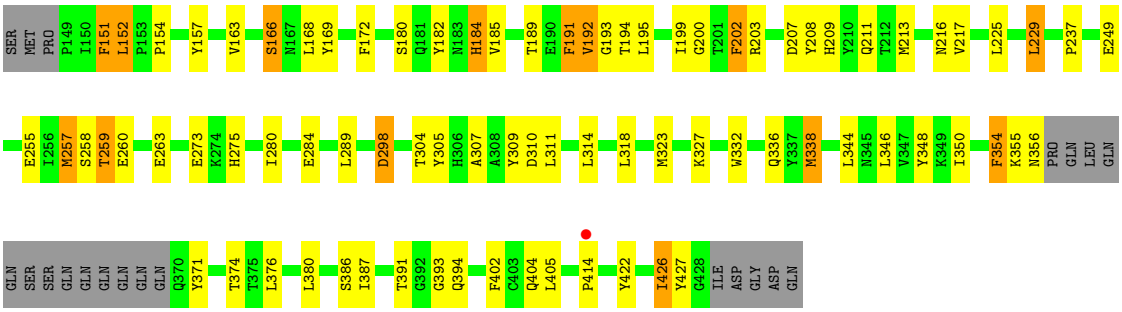
Chain E: 61% 27% • 7%





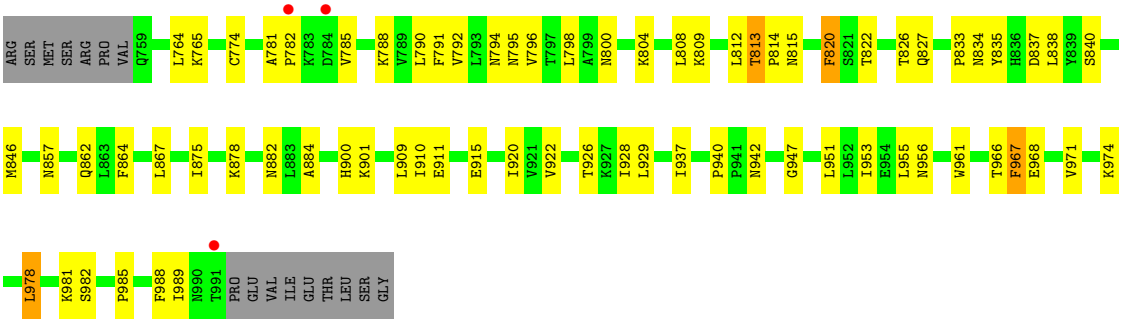
• Molecule 1: POLY(A) RIBONUCLEASE POP2

Chain F:



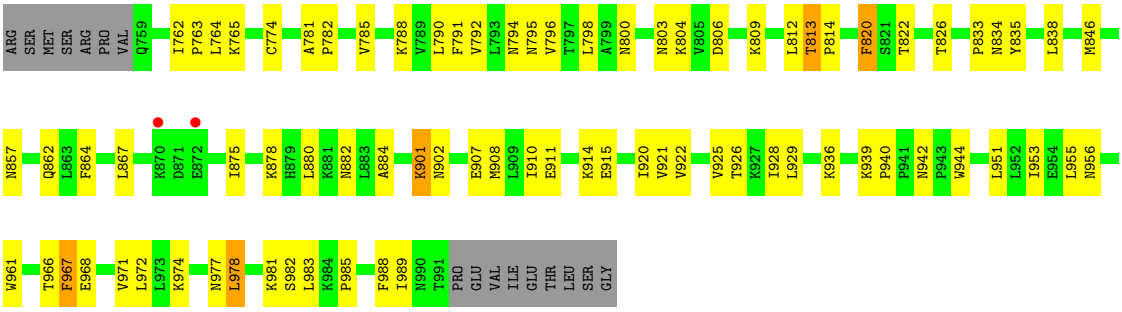
• Molecule 2: GENERAL NEGATIVE REGULATOR OF TRANSCRIPTION SUBUNIT 1

Chain B:



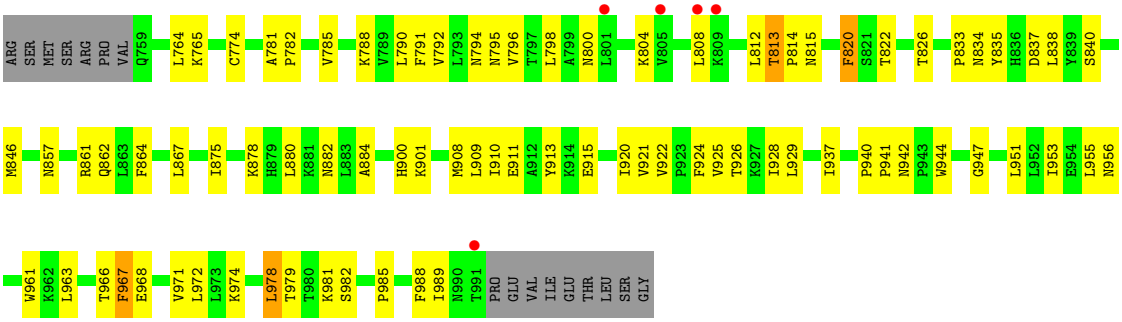
• Molecule 2: GENERAL NEGATIVE REGULATOR OF TRANSCRIPTION SUBUNIT 1

Chain G:



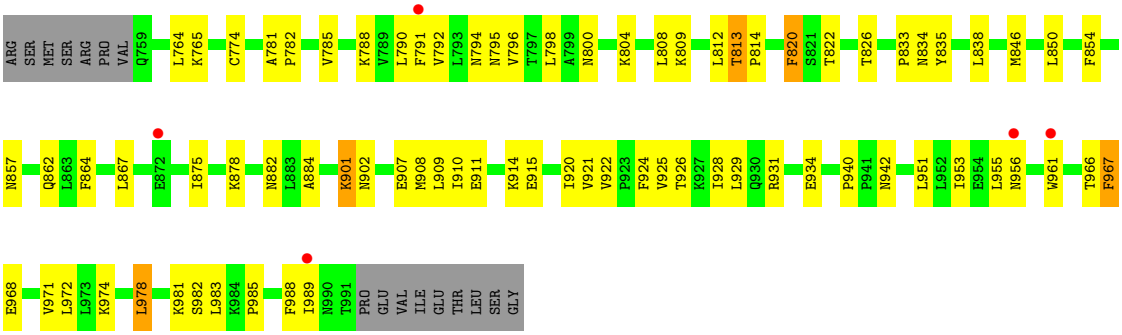
• Molecule 2: GENERAL NEGATIVE REGULATOR OF TRANSCRIPTION SUBUNIT 1

Chain H:



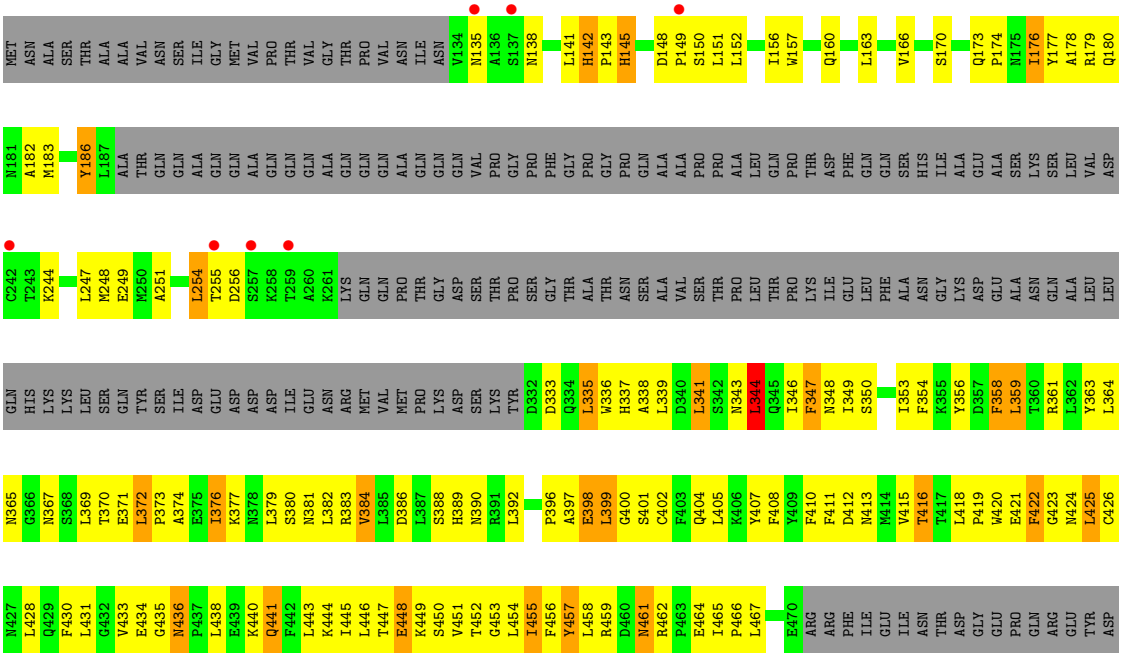
- Molecule 2: GENERAL NEGATIVE REGULATOR OF TRANSCRIPTION SUBUNIT 1

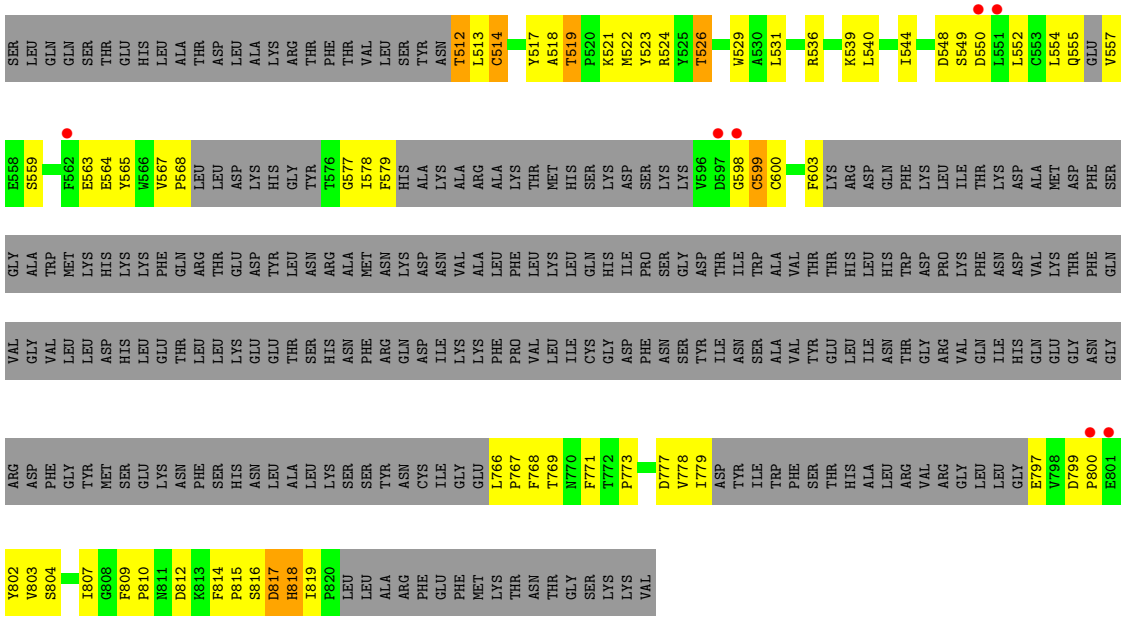
Chain I:



- Molecule 3: GLUCOSE-REPRESSIBLE ALCOHOL DEHYDROGENASE TRANSCRIPTIONAL EFFECTOR

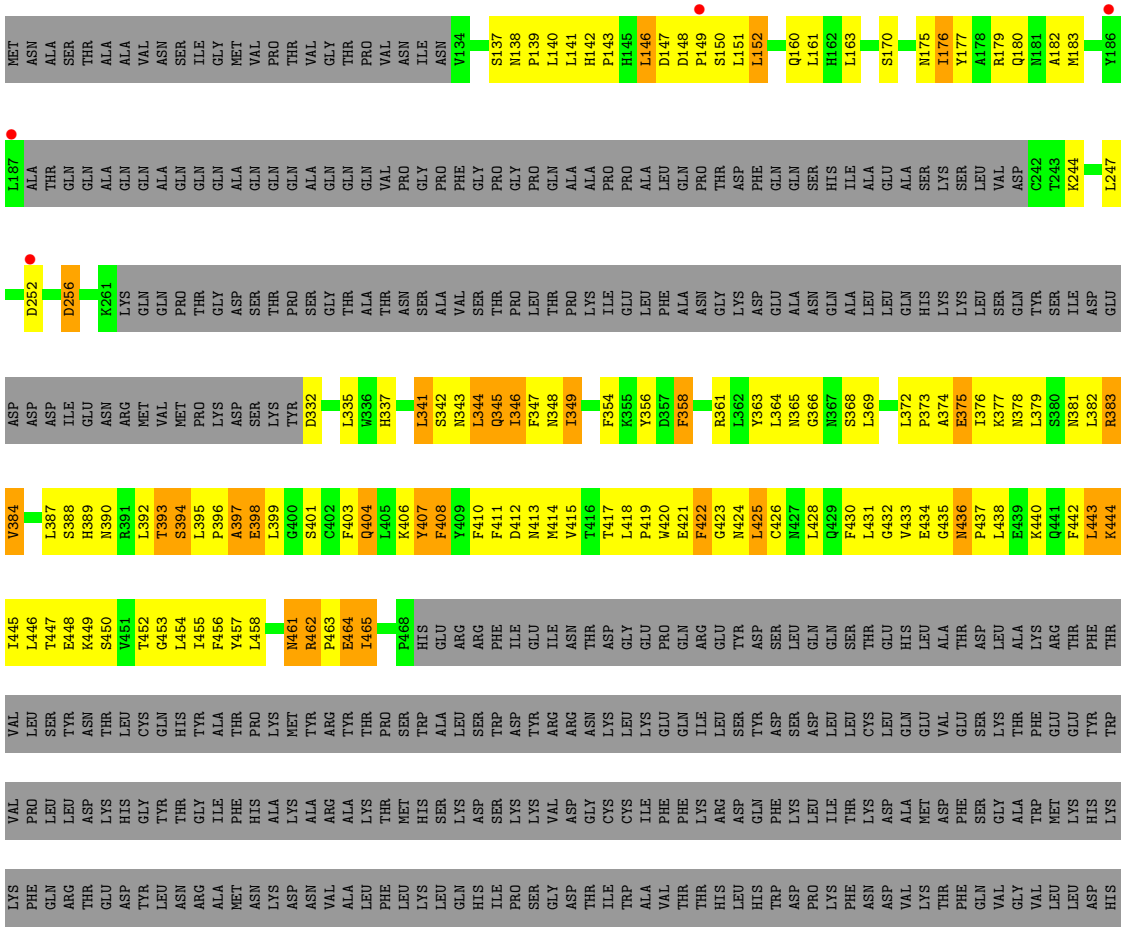
Chain D:

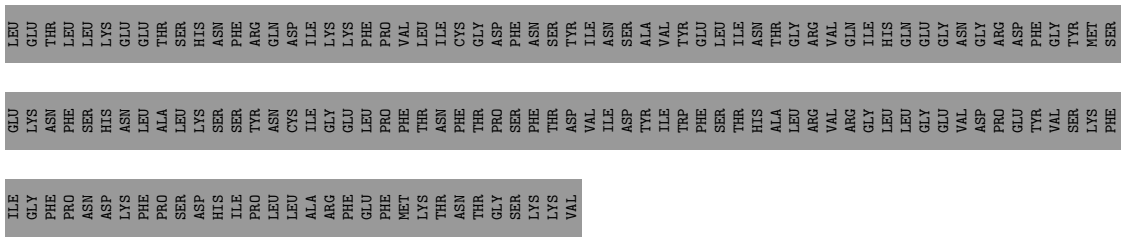




• Molecule 3: GLUCOSE-REPRESSIBLE ALCOHOL DEHYDROGENASE TRANSCRIPTIONAL EFFECTOR

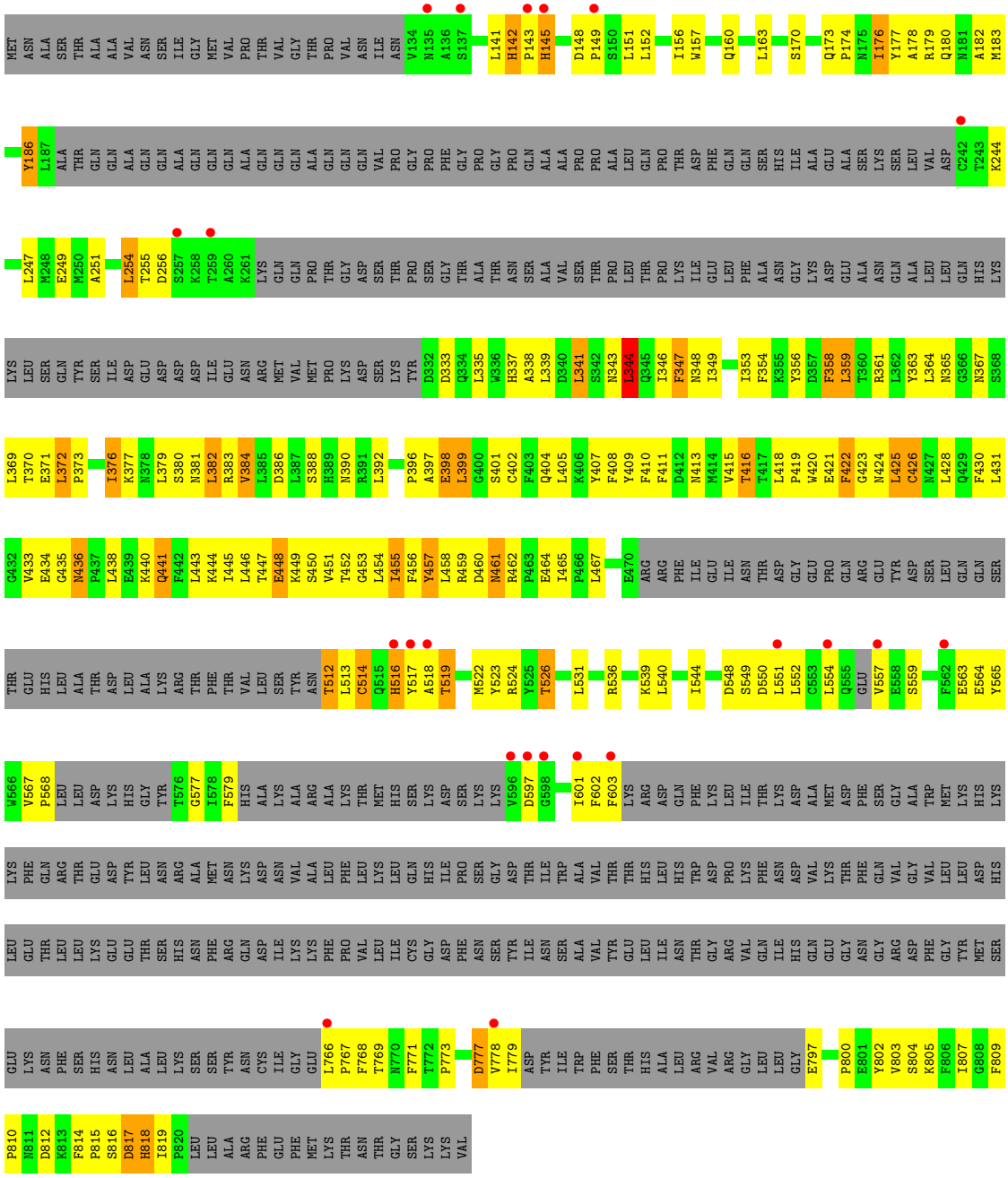
Chain J:





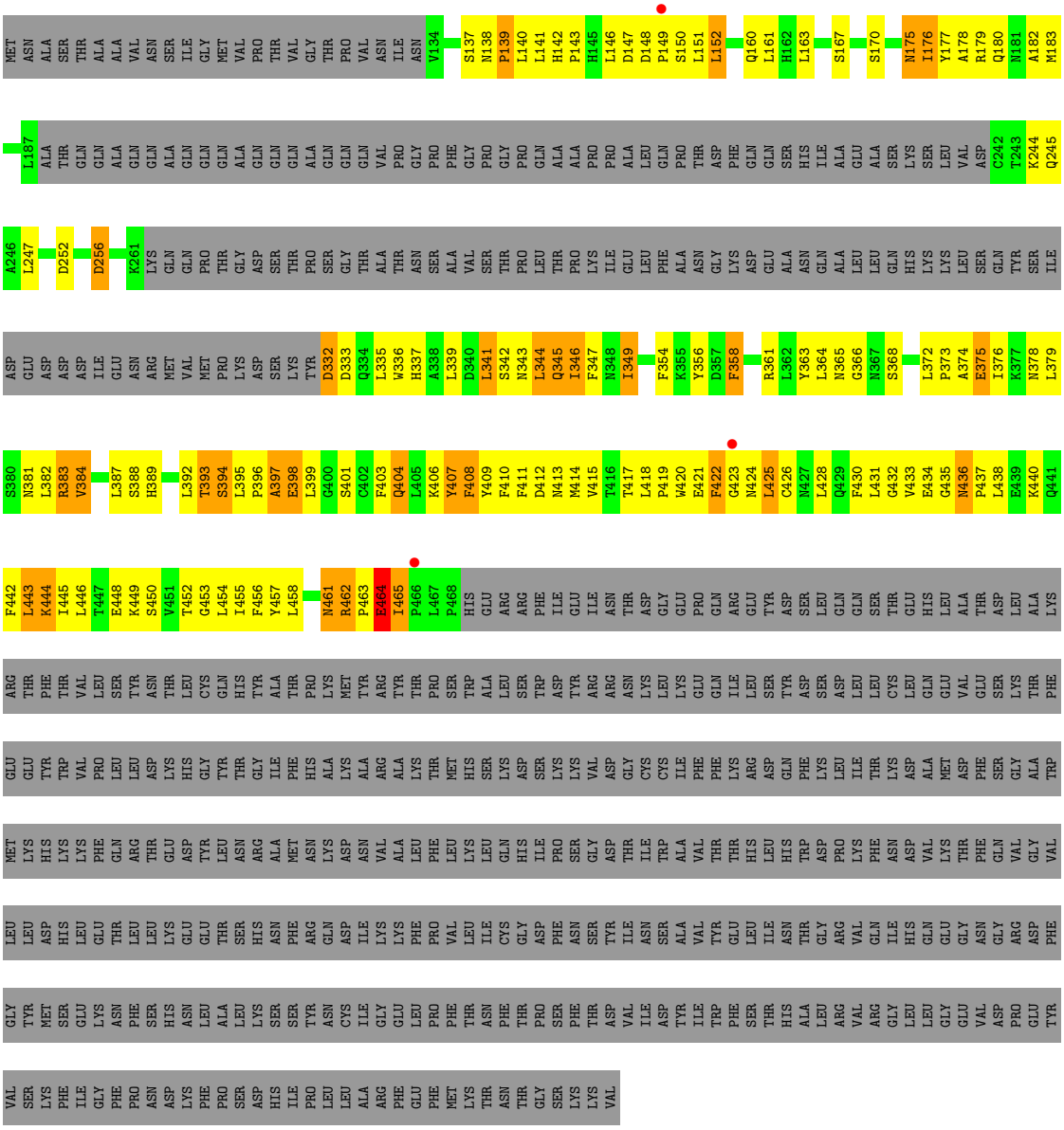
• Molecule 3: GLUCOSE-REPRESSIBLE ALCOHOL DEHYDROGENASE TRANSCRIPTIONAL EFFECTOR

Chain K:



• Molecule 3: GLUCOSE-REPRESSIBLE ALCOHOL DEHYDROGENASE TRANSCRIPTIONAL EFFECTOR

Chain L: 11% 14% • 71%



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	122.65Å 122.91Å 126.42Å 89.47° 89.74° 64.22°	Depositor
Resolution (Å)	47.95 – 3.41 48.23 – 3.28	Depositor EDS
% Data completeness (in resolution range)	97.1 (47.95-3.41) 97.4 (48.23-3.28)	Depositor EDS
R_{merge}	0.01	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.29 (at 3.25Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.7.1_743)	Depositor
R, R_{free}	0.233 , 0.270 0.226 , 0.264	Depositor DCC
R_{free} test set	4942 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	77.9	Xtriage
Anisotropy	0.333	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 72.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	0.026 for -h,-k,l 0.018 for k,h,-l 0.022 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	24298	wwPDB-VP
Average B, all atoms (Å^2)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.27% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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	0.56	0/2231	0.67	0/3028
1	C	0.54	0/2235	0.67	0/3032
1	E	0.50	0/2235	0.66	0/3033
1	F	0.52	0/2231	0.66	0/3028
2	B	0.43	0/1908	0.58	0/2588
2	G	0.42	0/1908	0.57	0/2588
2	H	0.43	0/1908	0.58	0/2588
2	I	0.44	0/1908	0.58	0/2588
3	D	0.53	0/2520	0.76	2/3446 (0.1%)
3	J	0.62	1/1640 (0.1%)	0.94	4/2240 (0.2%)
3	K	0.54	1/2535 (0.0%)	0.76	1/3463 (0.0%)
3	L	0.63	2/1640 (0.1%)	0.94	3/2240 (0.1%)
All	All	0.52	4/24899 (0.0%)	0.71	10/33862 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	C	0	1
1	E	0	1
3	D	0	1
3	J	0	1
3	K	0	1
3	L	0	2
All	All	0	8

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L	462	ARG	C-N	8.80	1.50	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	J	462	ARG	C-N	8.53	1.50	1.34
3	L	332	ASP	CA-CB	5.73	1.66	1.53
3	K	426	CYS	CB-SG	5.22	1.91	1.82

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	L	462	ARG	O-C-N	13.09	145.96	121.10
3	J	462	ARG	O-C-N	12.95	145.70	121.10
3	J	462	ARG	CA-C-N	-9.27	91.15	117.10
3	L	462	ARG	CA-C-N	-9.18	91.41	117.10
3	J	397	ALA	N-CA-C	-6.26	94.10	111.00
3	L	397	ALA	N-CA-C	-5.94	94.96	111.00
3	K	462	ARG	N-CA-C	-5.56	95.99	111.00
3	D	462	ARG	N-CA-C	-5.55	96.01	111.00
3	J	462	ARG	C-N-CD	5.11	139.13	128.40
3	D	335	LEU	N-CA-C	5.07	124.68	111.00

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	194	THR	Peptide
1	C	194	THR	Peptide
3	D	344	LEU	Peptide
1	E	194	THR	Peptide
3	J	332	ASP	Peptide
3	K	344	LEU	Peptide
3	L	332	ASP	Peptide
3	L	464	GLU	Mainchain

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	2170	0	2083	87	0
1	C	2174	0	2094	94	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	2174	0	2089	86	1
1	F	2170	0	2083	74	1
2	B	1869	0	1936	49	0
2	G	1869	0	1936	51	1
2	H	1869	0	1936	62	0
2	I	1869	0	1936	50	1
3	D	2456	0	2268	226	0
3	J	1604	0	1505	145	1
3	K	2470	0	2293	204	0
3	L	1604	0	1505	157	1
All	All	24298	0	23664	1240	3

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 26.

All (1240) 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:D:176:ILE:HD11	3:D:343:ASN:HD22	1.20	1.04
3:J:422:PHE:HD1	3:J:422:PHE:O	1.42	1.00
3:K:176:ILE:HD11	3:K:343:ASN:HD22	1.21	1.00
3:K:567:VAL:HG13	3:K:568:PRO:HD3	1.41	0.99
3:D:424:ASN:HD21	3:D:807:ILE:HG21	1.29	0.98
3:L:422:PHE:HD1	3:L:422:PHE:O	1.43	0.98
3:D:567:VAL:HG13	3:D:568:PRO:HD3	1.42	0.97
3:J:150:SER:HA	3:J:152:LEU:HD12	1.49	0.95
3:K:424:ASN:HD21	3:K:807:ILE:HG21	1.32	0.94
3:L:150:SER:HA	3:L:152:LEU:HD12	1.50	0.94
1:C:287:GLN:NE2	2:H:947:GLY:HA3	1.84	0.91
3:K:445:ILE:O	3:K:449:LYS:HB2	1.73	0.89
3:L:422:PHE:CB	3:L:425:LEU:HG	2.02	0.89
3:J:422:PHE:O	3:J:422:PHE:CD1	2.25	0.88
1:E:197:ARG:HG2	3:L:175:ASN:ND2	1.88	0.88
3:K:422:PHE:HB3	3:K:425:LEU:HG	1.56	0.88
3:D:422:PHE:HB3	3:D:425:LEU:HG	1.56	0.88
1:E:197:ARG:HG2	3:L:175:ASN:HD22	1.36	0.88
1:E:197:ARG:CG	3:L:175:ASN:HD22	1.84	0.88
3:J:422:PHE:CB	3:J:425:LEU:HG	2.04	0.88
3:D:176:ILE:HD11	3:D:343:ASN:ND2	1.90	0.87
3:D:445:ILE:O	3:D:449:LYS:HB2	1.75	0.87
3:K:579:PHE:HD1	3:K:579:PHE:O	1.55	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:176:ILE:HD11	3:K:343:ASN:ND2	1.91	0.86
3:L:422:PHE:O	3:L:422:PHE:CD1	2.27	0.86
3:D:422:PHE:HA	3:D:424:ASN:N	1.90	0.86
3:D:392:LEU:HB2	3:D:413:ASN:HD22	1.41	0.86
3:D:163:LEU:HD11	3:D:249:GLU:HA	1.58	0.85
3:K:163:LEU:HD11	3:K:249:GLU:HA	1.58	0.85
3:K:392:LEU:HB2	3:K:413:ASN:HD22	1.42	0.85
3:D:567:VAL:HG13	3:D:568:PRO:CD	2.07	0.84
3:K:579:PHE:O	3:K:579:PHE:CD1	2.31	0.84
3:K:567:VAL:HG13	3:K:568:PRO:CD	2.08	0.84
3:K:349:ILE:HG21	3:K:353:ILE:HD11	1.59	0.83
1:F:202:PHE:CE2	1:F:208:TYR:HD1	1.96	0.83
3:J:170:SER:HB3	3:J:176:ILE:HD13	1.61	0.83
1:C:203:ARG:HH22	3:K:333:ASP:CB	1.92	0.82
1:A:426:ILE:HG22	1:A:427:TYR:H	1.44	0.82
1:C:169:TYR:OH	1:C:284:GLU:OE1	1.98	0.82
3:K:424:ASN:HD21	3:K:807:ILE:CG2	1.94	0.81
1:E:169:TYR:OH	1:E:284:GLU:OE1	1.99	0.80
3:D:424:ASN:HD21	3:D:807:ILE:CG2	1.94	0.80
3:K:422:PHE:HA	3:K:424:ASN:N	1.95	0.80
3:J:419:PRO:HD2	3:J:422:PHE:CE1	2.14	0.80
1:A:169:TYR:OH	1:A:284:GLU:OE1	1.99	0.80
3:L:170:SER:HB3	3:L:176:ILE:HD13	1.63	0.80
3:D:418:LEU:HB3	3:D:422:PHE:HE1	1.46	0.80
3:L:137:SER:O	3:L:139:PRO:HD3	1.80	0.80
3:D:766:LEU:HG	3:D:767:PRO:HD2	1.62	0.80
3:J:449:LYS:HB3	3:J:453:GLY:HA3	1.64	0.80
3:K:418:LEU:HB3	3:K:422:PHE:HE1	1.47	0.80
3:D:349:ILE:HG21	3:D:353:ILE:HD11	1.62	0.79
1:F:169:TYR:OH	1:F:284:GLU:OE1	2.00	0.79
3:D:397:ALA:O	3:D:399:LEU:N	2.15	0.79
1:E:305:TYR:OH	1:E:371:TYR:O	1.99	0.79
1:A:287:GLN:NE2	2:B:947:GLY:HA3	1.97	0.79
3:J:137:SER:O	3:J:139:PRO:HD3	1.82	0.79
1:E:202:PHE:CE2	1:E:208:TYR:HD1	2.01	0.78
1:E:213:MET:HG3	1:E:309:TYR:CD1	2.18	0.78
1:F:305:TYR:OH	1:F:371:TYR:O	2.01	0.78
1:C:305:TYR:OH	1:C:371:TYR:O	2.01	0.78
1:F:194:THR:HG23	1:F:194:THR:O	1.81	0.78
3:L:150:SER:HA	3:L:152:LEU:CD1	2.12	0.78
1:A:305:TYR:OH	1:A:371:TYR:O	2.02	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:426:ILE:HG22	1:C:427:TYR:H	1.48	0.78
1:F:213:MET:HG3	1:F:309:TYR:CD1	2.19	0.78
3:J:150:SER:HA	3:J:152:LEU:CD1	2.13	0.77
1:E:426:ILE:HG22	1:E:427:TYR:H	1.49	0.77
3:K:397:ALA:O	3:K:399:LEU:N	2.17	0.77
3:L:422:PHE:HB2	3:L:425:LEU:HG	1.65	0.76
3:K:399:LEU:O	3:K:402:CYS:HB2	1.86	0.76
1:C:202:PHE:CE2	1:C:208:TYR:HD1	2.04	0.76
3:L:376:ILE:HD12	3:L:379:LEU:HD12	1.66	0.76
1:A:203:ARG:HH22	3:D:333:ASP:CB	1.99	0.76
3:D:372:LEU:HD21	3:D:376:ILE:HD13	1.68	0.76
3:L:419:PRO:HD2	3:L:422:PHE:CE1	2.20	0.75
3:L:449:LYS:HB3	3:L:453:GLY:HA3	1.68	0.75
3:K:766:LEU:HG	3:K:767:PRO:HD2	1.67	0.75
3:D:399:LEU:O	3:D:402:CYS:HB2	1.87	0.75
1:A:189:THR:OG1	1:A:310:ASP:OD1	2.04	0.75
2:I:790:LEU:O	2:I:794:ASN:ND2	2.19	0.75
3:J:422:PHE:HB3	3:J:425:LEU:HG	1.66	0.75
3:K:773:PRO:HD3	3:K:807:ILE:O	1.87	0.75
3:K:349:ILE:HG21	3:K:353:ILE:CD1	2.15	0.75
1:C:189:THR:OG1	1:C:310:ASP:OD1	2.04	0.75
1:F:426:ILE:HG22	1:F:427:TYR:H	1.52	0.74
3:D:349:ILE:HG21	3:D:353:ILE:CD1	2.16	0.74
3:J:422:PHE:HA	3:J:424:ASN:N	2.03	0.74
3:L:383:ARG:CZ	3:L:404:GLN:HG2	2.18	0.74
3:D:773:PRO:HD3	3:D:807:ILE:O	1.88	0.74
1:E:203:ARG:HH22	3:L:333:ASP:CB	2.00	0.73
3:J:422:PHE:HB2	3:J:425:LEU:HG	1.69	0.73
3:D:397:ALA:O	3:D:398:GLU:HG2	1.88	0.73
1:F:189:THR:OG1	1:F:310:ASP:OD1	2.05	0.73
1:F:202:PHE:CE2	1:F:208:TYR:CD1	2.76	0.73
3:J:442:PHE:HE1	3:J:458:LEU:HD21	1.53	0.73
3:L:422:PHE:HB3	3:L:425:LEU:HG	1.68	0.73
1:E:195:LEU:HA	1:E:216:ASN:OD1	1.88	0.73
3:K:428:LEU:HD21	3:K:431:LEU:HB2	1.69	0.73
1:F:191:PHE:CZ	1:F:309:TYR:HD2	2.05	0.73
3:J:383:ARG:CZ	3:J:404:GLN:HG2	2.19	0.73
3:K:397:ALA:O	3:K:398:GLU:HG2	1.89	0.73
1:A:191:PHE:CZ	1:A:309:TYR:HD2	2.07	0.73
1:A:195:LEU:HA	1:A:216:ASN:OD1	1.88	0.73
3:K:422:PHE:HB2	3:K:425:LEU:HD11	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:446:LEU:HD12	3:D:450:SER:O	1.87	0.72
3:D:766:LEU:CG	3:D:767:PRO:HD2	2.18	0.72
3:K:372:LEU:HD21	3:K:376:ILE:HD13	1.71	0.72
3:J:420:TRP:CE2	3:J:463:PRO:HD3	2.24	0.72
3:L:442:PHE:HE1	3:L:458:LEU:HD21	1.53	0.72
3:D:578:ILE:HG22	3:D:579:PHE:N	2.04	0.72
1:E:191:PHE:CZ	1:E:309:TYR:HD2	2.06	0.71
3:K:422:PHE:HB3	3:K:425:LEU:CG	2.19	0.71
3:L:422:PHE:HA	3:L:424:ASN:N	2.06	0.71
3:D:578:ILE:HG22	3:D:579:PHE:H	1.56	0.71
3:L:148:ASP:HB3	3:L:149:PRO:C	2.10	0.71
3:D:577:GLY:C	3:D:578:ILE:HD12	2.11	0.71
1:E:189:THR:OG1	1:E:310:ASP:OD1	2.06	0.71
1:E:202:PHE:CE2	1:E:208:TYR:CD1	2.78	0.71
1:A:202:PHE:CE2	1:A:208:TYR:HD1	2.09	0.71
2:B:790:LEU:O	2:B:794:ASN:ND2	2.23	0.71
3:J:397:ALA:O	3:J:398:GLU:HG2	1.91	0.71
3:L:143:PRO:HG3	3:L:443:LEU:HD11	1.71	0.71
1:C:176:ARG:HD3	2:H:900:HIS:HB3	1.73	0.71
3:K:411:PHE:HD1	3:K:434:GLU:O	1.74	0.71
1:C:287:GLN:HE22	2:H:947:GLY:HA3	1.53	0.71
3:J:148:ASP:HB3	3:J:149:PRO:C	2.10	0.71
2:H:790:LEU:O	2:H:794:ASN:ND2	2.24	0.70
2:G:790:LEU:O	2:G:794:ASN:ND2	2.23	0.70
3:D:422:PHE:HB2	3:D:425:LEU:HD11	1.72	0.70
3:D:428:LEU:HD21	3:D:431:LEU:HB2	1.72	0.70
3:D:440:LYS:O	3:D:444:LYS:HG3	1.91	0.70
3:K:461:ASN:OD1	3:K:461:ASN:N	2.24	0.70
1:C:191:PHE:CZ	1:C:309:TYR:HD2	2.10	0.70
3:D:411:PHE:HD1	3:D:434:GLU:O	1.75	0.70
3:D:529:TRP:HB3	2:H:913:TYR:CE2	2.27	0.70
3:D:766:LEU:HD21	3:D:797:GLU:N	2.07	0.70
2:G:833:PRO:HD3	2:G:882:ASN:ND2	2.07	0.70
3:D:422:PHE:CB	3:D:425:LEU:HG	2.22	0.69
3:L:383:ARG:NH1	3:L:404:GLN:HG2	2.06	0.69
3:L:419:PRO:O	3:L:420:TRP:HB2	1.92	0.69
1:C:195:LEU:HA	1:C:216:ASN:OD1	1.91	0.69
3:D:422:PHE:HB3	3:D:425:LEU:CG	2.21	0.69
3:J:383:ARG:NH1	3:J:404:GLN:HG2	2.06	0.69
3:D:579:PHE:CZ	3:D:598:GLY:HA3	2.27	0.69
3:L:397:ALA:O	3:L:398:GLU:HG2	1.93	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:433:VAL:O	3:L:435:GLY:HA2	1.91	0.69
3:D:428:LEU:HB3	3:D:455:ILE:HD11	1.74	0.69
3:K:422:PHE:CB	3:K:425:LEU:HG	2.22	0.69
3:J:358:PHE:HD1	3:J:358:PHE:H	1.40	0.68
1:C:213:MET:HG3	1:C:309:TYR:CD1	2.28	0.68
3:J:376:ILE:HD12	3:J:379:LEU:HD12	1.73	0.68
3:K:766:LEU:CG	3:K:767:PRO:HD2	2.23	0.68
3:K:440:LYS:O	3:K:444:LYS:HG3	1.93	0.68
2:G:967:PHE:O	2:G:971:VAL:HG23	1.93	0.68
1:C:305:TYR:HD1	1:C:344:LEU:HB3	1.57	0.68
3:D:344:LEU:O	3:D:346:ILE:HG13	1.93	0.68
3:L:347:PHE:HD1	3:L:368:SER:HB2	1.58	0.68
3:D:422:PHE:HA	3:D:424:ASN:H	1.57	0.68
3:D:461:ASN:OD1	3:D:461:ASN:N	2.27	0.68
3:L:374:ALA:HB1	3:L:398:GLU:OE2	1.93	0.68
3:J:244:LYS:O	3:J:247:LEU:N	2.26	0.67
3:D:361:ARG:HA	3:D:384:VAL:HG23	1.77	0.67
3:J:374:ALA:HB1	3:J:398:GLU:OE2	1.94	0.67
3:K:428:LEU:HB3	3:K:455:ILE:HD11	1.77	0.67
3:K:344:LEU:O	3:K:346:ILE:HG13	1.94	0.67
3:L:354:PHE:CZ	3:L:373:PRO:HG2	2.29	0.66
2:H:884:ALA:HB1	2:H:928:ILE:HG13	1.77	0.66
1:E:305:TYR:HD1	1:E:344:LEU:HB3	1.58	0.66
3:J:347:PHE:HD1	3:J:368:SER:HB2	1.59	0.66
3:K:446:LEU:HD12	3:K:450:SER:O	1.95	0.66
1:A:176:ARG:HD3	2:B:900:HIS:HB3	1.77	0.66
3:D:335:LEU:O	3:D:337:HIS:CE1	2.49	0.66
3:L:244:LYS:O	3:L:247:LEU:N	2.28	0.66
2:H:781:ALA:HB1	2:H:785:VAL:HB	1.78	0.66
3:K:335:LEU:O	3:K:337:HIS:CE1	2.49	0.65
3:K:361:ARG:HA	3:K:384:VAL:HG23	1.78	0.65
3:D:142:HIS:CD2	3:D:142:HIS:H	2.12	0.65
3:D:397:ALA:C	3:D:399:LEU:H	1.99	0.65
3:J:396:PRO:HD2	3:J:399:LEU:HD12	1.77	0.65
3:K:142:HIS:CD2	3:K:142:HIS:H	2.13	0.65
3:L:396:PRO:HD2	3:L:399:LEU:HD12	1.78	0.65
1:E:194:THR:O	1:E:194:THR:HG23	1.97	0.65
3:L:345:GLN:N	3:L:345:GLN:OE1	2.30	0.65
3:L:358:PHE:HD1	3:L:358:PHE:H	1.44	0.65
3:K:540:LEU:HD23	3:K:815:PRO:HG2	1.79	0.65
3:J:346:ILE:O	3:J:346:ILE:HG22	1.95	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:766:LEU:HD21	3:K:797:GLU:N	2.12	0.65
3:D:251:ALA:O	3:D:254:LEU:N	2.29	0.64
2:I:967:PHE:O	2:I:971:VAL:HG23	1.97	0.64
1:A:213:MET:HG3	1:A:309:TYR:CD1	2.32	0.64
3:D:346:ILE:HB	3:D:367:ASN:HD22	1.63	0.64
2:H:833:PRO:HD3	2:H:882:ASN:ND2	2.11	0.64
3:J:354:PHE:CZ	3:J:373:PRO:HG2	2.32	0.64
3:L:420:TRP:CE2	3:L:463:PRO:HD3	2.32	0.64
1:A:287:GLN:HE22	2:B:947:GLY:HA3	1.62	0.64
1:A:305:TYR:HD1	1:A:344:LEU:HB3	1.61	0.64
3:D:157:TRP:HZ3	3:D:443:LEU:HD22	1.62	0.64
3:J:419:PRO:HD2	3:J:422:PHE:HE1	1.62	0.64
3:J:160:GLN:HE22	3:J:432:GLY:HA2	1.63	0.64
2:B:922:VAL:O	2:B:926:THR:HG23	1.98	0.64
3:L:346:ILE:O	3:L:346:ILE:HG22	1.96	0.64
3:J:440:LYS:HA	3:J:443:LEU:HB2	1.79	0.64
2:B:833:PRO:HD3	2:B:882:ASN:ND2	2.13	0.64
2:I:833:PRO:HD3	2:I:882:ASN:ND2	2.13	0.64
3:K:397:ALA:C	3:K:399:LEU:H	2.01	0.64
3:J:433:VAL:O	3:J:435:GLY:HA2	1.98	0.63
3:K:183:MET:O	3:K:186:TYR:HB3	1.98	0.63
3:L:440:LYS:HA	3:L:443:LEU:HB2	1.79	0.63
3:J:143:PRO:HG3	3:J:443:LEU:HD11	1.78	0.63
3:K:518:ALA:O	3:K:531:LEU:HD11	1.97	0.63
2:G:922:VAL:O	2:G:926:THR:HG23	1.98	0.63
3:L:160:GLN:HE22	3:L:432:GLY:HA2	1.64	0.63
1:C:191:PHE:HD1	1:C:191:PHE:N	1.96	0.63
3:D:766:LEU:CD1	3:D:767:PRO:HD2	2.29	0.63
3:K:550:ASP:O	3:K:603:PHE:HA	1.98	0.63
3:D:183:MET:O	3:D:186:TYR:HB3	1.98	0.63
3:D:518:ALA:O	3:D:531:LEU:HD11	1.97	0.63
3:K:513:LEU:HD12	3:K:816:SER:HA	1.80	0.63
3:L:417:THR:HG23	3:L:442:PHE:CE2	2.34	0.63
2:B:875:ILE:HD12	2:B:920:ILE:HG12	1.79	0.63
1:F:191:PHE:N	1:F:191:PHE:HD1	1.96	0.63
3:J:403:PHE:CD1	3:J:404:GLN:N	2.67	0.63
2:I:781:ALA:HB1	2:I:785:VAL:HB	1.78	0.63
1:C:355:LYS:O	1:C:355:LYS:HG3	1.97	0.63
3:D:540:LEU:HD23	3:D:815:PRO:HG2	1.81	0.62
2:I:956:ASN:HD21	2:I:966:THR:HG23	1.63	0.62
2:B:884:ALA:HB1	2:B:928:ILE:HG13	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:202:PHE:CE2	1:C:208:TYR:CD1	2.85	0.62
2:B:781:ALA:HB1	2:B:785:VAL:HB	1.82	0.62
3:K:766:LEU:CD1	3:K:767:PRO:HD2	2.30	0.62
3:D:179:ARG:O	3:D:182:ALA:HB3	1.99	0.62
3:D:349:ILE:HD11	3:D:369:LEU:HD21	1.81	0.62
3:D:578:ILE:CG2	3:D:579:PHE:H	2.12	0.62
1:E:197:ARG:HG3	3:L:175:ASN:HD22	1.63	0.62
3:D:419:PRO:HD2	3:D:422:PHE:CZ	2.34	0.62
3:K:157:TRP:HZ3	3:K:443:LEU:HD22	1.64	0.62
3:K:419:PRO:HD2	3:K:422:PHE:CE1	2.35	0.62
3:K:422:PHE:HA	3:K:424:ASN:H	1.64	0.62
3:K:766:LEU:HD11	3:K:797:GLU:CB	2.29	0.62
2:B:967:PHE:O	2:B:971:VAL:HG23	2.00	0.62
3:J:419:PRO:HD2	3:J:422:PHE:CZ	2.33	0.62
3:K:433:VAL:O	3:K:435:GLY:HA2	1.99	0.62
3:D:513:LEU:HD12	3:D:816:SER:HA	1.82	0.62
3:K:577:GLY:HA3	3:K:602:PHE:CD1	2.34	0.62
3:D:464:GLU:O	3:D:465:ILE:HD13	1.99	0.62
1:C:192:VAL:HG11	1:C:257:MET:HG2	1.82	0.61
3:D:160:GLN:NE2	3:D:430:PHE:CE1	2.68	0.61
3:D:433:VAL:O	3:D:435:GLY:HA2	2.00	0.61
1:A:192:VAL:HG11	1:A:257:MET:HG2	1.82	0.61
3:L:403:PHE:CD1	3:L:404:GLN:N	2.69	0.61
3:K:420:TRP:CZ3	3:K:461:ASN:O	2.54	0.61
1:C:191:PHE:N	1:C:191:PHE:CD1	2.67	0.61
1:F:195:LEU:HA	1:F:216:ASN:OD1	2.01	0.61
1:F:305:TYR:HD1	1:F:344:LEU:HB3	1.63	0.61
1:F:154:PRO:HG2	1:F:157:TYR:CD1	2.36	0.61
2:I:884:ALA:HB1	2:I:928:ILE:HG13	1.82	0.61
3:K:449:LYS:HB3	3:K:453:GLY:HA3	1.83	0.61
1:F:192:VAL:HG11	1:F:257:MET:HG2	1.83	0.61
2:H:967:PHE:O	2:H:971:VAL:HG23	2.01	0.61
3:L:379:LEU:O	3:L:382:LEU:HB2	2.01	0.61
3:D:419:PRO:HD2	3:D:422:PHE:CE1	2.36	0.61
3:D:420:TRP:CZ3	3:D:461:ASN:O	2.54	0.61
3:J:396:PRO:O	3:J:399:LEU:HB2	2.00	0.61
3:K:251:ALA:O	3:K:254:LEU:N	2.33	0.61
3:K:419:PRO:HD2	3:K:422:PHE:CZ	2.36	0.61
3:K:769:THR:HG23	3:K:778:VAL:HG13	1.82	0.61
3:L:423:GLY:HA3	3:L:455:ILE:HG23	1.81	0.60
2:H:875:ILE:HD12	2:H:920:ILE:HG12	1.81	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:512:THR:CG2	3:K:512:THR:O	2.48	0.60
3:L:396:PRO:O	3:L:399:LEU:HB2	2.00	0.60
2:I:922:VAL:O	2:I:926:THR:HG23	2.02	0.60
3:J:345:GLN:N	3:J:345:GLN:OE1	2.34	0.60
1:E:191:PHE:HD1	1:E:191:PHE:N	1.99	0.60
3:K:349:ILE:HD11	3:K:369:LEU:HD21	1.83	0.60
3:K:420:TRP:O	3:K:422:PHE:O	2.19	0.60
3:D:440:LYS:HA	3:D:443:LEU:HD12	1.83	0.60
1:F:207:ASP:O	1:F:211:GLN:HG2	2.02	0.60
2:G:781:ALA:HB1	2:G:785:VAL:HB	1.83	0.60
3:D:449:LYS:HB3	3:D:453:GLY:HA3	1.84	0.60
1:F:191:PHE:HD1	1:F:191:PHE:H	1.48	0.60
3:L:397:ALA:O	3:L:398:GLU:CG	2.49	0.60
3:D:766:LEU:HD11	3:D:797:GLU:CB	2.31	0.60
3:K:411:PHE:CD1	3:K:434:GLU:O	2.54	0.60
2:G:956:ASN:HD21	2:G:966:THR:HG23	1.66	0.59
2:H:922:VAL:O	2:H:926:THR:HG23	2.03	0.59
2:B:782:PRO:HG2	2:B:785:VAL:HG23	1.82	0.59
3:K:440:LYS:HA	3:K:443:LEU:HD12	1.84	0.59
3:K:346:ILE:HB	3:K:367:ASN:HD22	1.67	0.59
1:F:191:PHE:N	1:F:191:PHE:CD1	2.68	0.59
3:D:180:GLN:OE1	3:D:244:LYS:HA	2.02	0.59
2:B:956:ASN:HD21	2:B:966:THR:HG23	1.66	0.59
3:D:411:PHE:CD1	3:D:434:GLU:O	2.55	0.59
3:D:578:ILE:HD12	3:D:578:ILE:N	2.17	0.59
1:A:202:PHE:CE2	1:A:208:TYR:CD1	2.89	0.59
3:D:346:ILE:HB	3:D:367:ASN:ND2	2.17	0.59
3:D:424:ASN:ND2	3:D:807:ILE:HG21	2.11	0.59
3:D:769:THR:HG23	3:D:778:VAL:HG13	1.83	0.59
2:H:782:PRO:HG2	2:H:785:VAL:HG23	1.83	0.59
3:K:464:GLU:O	3:K:465:ILE:HD13	2.02	0.59
3:L:419:PRO:HD2	3:L:422:PHE:HE1	1.66	0.59
3:L:433:VAL:HB	3:L:438:LEU:HD11	1.85	0.59
1:E:202:PHE:CE1	3:L:336:TRP:HB3	2.38	0.58
1:C:151:PHE:CD1	1:C:151:PHE:C	2.76	0.58
1:F:191:PHE:HZ	1:F:309:TYR:HD2	1.51	0.58
3:D:512:THR:CG2	3:D:512:THR:O	2.51	0.58
3:D:768:PHE:CE2	3:D:771:PHE:HB2	2.38	0.58
2:H:956:ASN:HD21	2:H:966:THR:HG23	1.66	0.58
1:A:191:PHE:N	1:A:191:PHE:HD1	2.01	0.58
1:A:199:ILE:HB	3:D:338:ALA:HB3	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:953:ILE:HG22	2:B:985:PRO:HB3	1.86	0.58
3:K:422:PHE:HB2	3:K:425:LEU:CD1	2.31	0.58
3:K:516:HIS:O	3:K:516:HIS:ND1	2.37	0.58
3:L:177:TYR:CD2	3:L:363:TYR:CZ	2.91	0.58
3:D:423:GLY:H	3:D:458:LEU:HB2	1.67	0.58
2:G:834:ASN:HB2	2:G:835:TYR:CD1	2.39	0.58
3:K:347:PHE:H	3:K:347:PHE:HD1	1.50	0.58
2:B:955:LEU:HD23	2:B:989:ILE:HG13	1.85	0.58
3:J:417:THR:HG23	3:J:442:PHE:CE2	2.39	0.58
3:J:428:LEU:HD21	3:J:431:LEU:HB2	1.85	0.58
3:L:179:ARG:O	3:L:182:ALA:HB3	2.04	0.58
3:L:422:PHE:CB	3:L:425:LEU:CG	2.80	0.58
3:K:539:LYS:CB	3:K:815:PRO:HG3	2.33	0.58
2:H:955:LEU:HD23	2:H:989:ILE:HG13	1.85	0.58
3:K:148:ASP:HB3	3:K:149:PRO:C	2.24	0.58
1:A:298:ASP:OD1	1:A:298:ASP:N	2.35	0.58
1:E:191:PHE:HZ	1:E:309:TYR:HD2	1.51	0.58
3:J:177:TYR:CD2	3:J:363:TYR:CZ	2.92	0.58
3:K:512:THR:O	3:K:512:THR:HG23	2.04	0.58
1:A:191:PHE:N	1:A:191:PHE:CD1	2.72	0.57
3:D:455:ILE:HG22	3:D:456:PHE:N	2.19	0.57
3:J:397:ALA:C	3:J:399:LEU:H	2.06	0.57
3:J:433:VAL:HB	3:J:438:LEU:HD11	1.86	0.57
3:K:766:LEU:HD12	3:K:767:PRO:HD2	1.86	0.57
3:D:802:TYR:O	3:D:804:SER:O	2.21	0.57
1:E:191:PHE:N	1:E:191:PHE:CD1	2.70	0.57
3:J:179:ARG:O	3:J:182:ALA:HB3	2.05	0.57
2:G:798:LEU:HD12	2:G:838:LEU:HD13	1.85	0.57
1:C:199:ILE:HG22	1:C:200:GLY:H	1.69	0.57
2:G:800:ASN:ND2	2:G:804:LYS:HG3	2.20	0.57
1:A:151:PHE:CD1	1:A:151:PHE:C	2.78	0.57
1:A:257:MET:O	3:D:347:PHE:CD1	2.58	0.57
1:C:191:PHE:HD1	1:C:191:PHE:H	1.51	0.57
3:D:422:PHE:HB2	3:D:425:LEU:CD1	2.32	0.57
3:K:388:SER:HA	3:K:411:PHE:H	1.69	0.57
3:D:578:ILE:CG2	3:D:579:PHE:N	2.67	0.57
3:D:768:PHE:CD2	3:D:771:PHE:HB2	2.40	0.57
3:D:766:LEU:HD12	3:D:767:PRO:HD2	1.87	0.57
3:K:180:GLN:OE1	3:K:244:LYS:HA	2.04	0.57
3:D:354:PHE:CE2	3:D:373:PRO:HG2	2.40	0.57
3:D:539:LYS:CB	3:D:815:PRO:HG3	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:419:PRO:O	3:J:421:GLU:HG2	2.05	0.57
3:L:140:LEU:HG	3:L:437:PRO:HB3	1.86	0.57
3:D:422:PHE:CA	3:D:424:ASN:H	2.18	0.56
2:H:812:LEU:HD21	2:H:820:PHE:HD2	1.70	0.56
3:K:143:PRO:HD2	3:K:157:TRP:CH2	2.40	0.56
3:K:179:ARG:O	3:K:182:ALA:HB3	2.05	0.56
3:K:369:LEU:HD13	3:K:390:ASN:OD1	2.05	0.56
3:K:422:PHE:CD2	3:K:425:LEU:HD21	2.41	0.56
3:D:148:ASP:HB3	3:D:149:PRO:C	2.25	0.56
3:J:396:PRO:C	3:J:397:ALA:O	2.37	0.56
1:E:191:PHE:HD1	1:E:191:PHE:H	1.52	0.56
1:F:151:PHE:CD1	1:F:151:PHE:C	2.75	0.56
3:K:436:ASN:O	3:K:438:LEU:N	2.38	0.56
1:A:257:MET:O	3:D:347:PHE:HD1	1.88	0.56
3:D:444:LYS:HB3	2:H:963:LEU:HD12	1.87	0.56
2:G:910:ILE:HD11	2:G:988:PHE:HB3	1.88	0.56
2:I:875:ILE:HD12	2:I:920:ILE:HG12	1.88	0.56
3:K:354:PHE:CE2	3:K:373:PRO:HG2	2.41	0.56
2:G:782:PRO:HG2	2:G:785:VAL:HG23	1.86	0.56
2:G:834:ASN:HB2	2:G:835:TYR:CE1	2.41	0.56
2:G:884:ALA:HB1	2:G:928:ILE:HG13	1.87	0.56
3:J:397:ALA:O	3:J:398:GLU:CG	2.53	0.56
1:C:354:PHE:HD2	1:C:414:PRO:HB2	1.71	0.56
3:K:455:ILE:HG22	3:K:456:PHE:N	2.20	0.56
3:L:384:VAL:HG22	3:L:407:TYR:HB2	1.88	0.56
3:D:388:SER:HA	3:D:411:PHE:H	1.71	0.56
2:I:910:ILE:HD11	2:I:988:PHE:HB3	1.88	0.56
1:C:199:ILE:HB	3:K:338:ALA:HB3	1.87	0.56
3:D:523:TYR:CD1	3:D:523:TYR:N	2.72	0.56
1:F:193:GLY:C	1:F:195:LEU:HD23	2.26	0.56
1:F:194:THR:O	1:F:194:THR:CG2	2.52	0.56
3:L:422:PHE:HB2	3:L:425:LEU:CG	2.34	0.56
3:J:379:LEU:O	3:J:382:LEU:HB2	2.06	0.56
3:J:423:GLY:HA3	3:J:455:ILE:HG23	1.86	0.56
3:K:802:TYR:O	3:K:804:SER:O	2.24	0.56
3:D:392:LEU:HD12	3:D:413:ASN:ND2	2.21	0.55
3:D:415:VAL:H	3:D:436:ASN:HB3	1.71	0.55
1:E:354:PHE:HD1	1:E:354:PHE:N	2.04	0.55
1:A:207:ASP:O	1:A:211:GLN:HG2	2.06	0.55
2:G:875:ILE:HD12	2:G:920:ILE:HG12	1.88	0.55
3:K:160:GLN:NE2	3:K:430:PHE:CE1	2.73	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:381:ASN:O	3:K:383:ARG:NH1	2.39	0.55
3:K:768:PHE:CE2	3:K:771:PHE:HB2	2.42	0.55
3:D:416:THR:O	3:D:438:LEU:HD23	2.06	0.55
1:E:192:VAL:HG11	1:E:257:MET:HG2	1.89	0.55
1:E:213:MET:HG3	1:E:309:TYR:CE1	2.41	0.55
3:J:419:PRO:CD	3:J:422:PHE:CE1	2.89	0.55
1:E:151:PHE:CD1	1:E:151:PHE:C	2.77	0.55
1:E:354:PHE:HD2	1:E:414:PRO:HB2	1.72	0.55
2:H:940:PRO:HA	2:H:942:ASN:H	1.72	0.55
3:K:142:HIS:CD2	3:K:142:HIS:N	2.75	0.55
3:K:423:GLY:H	3:K:458:LEU:HB2	1.71	0.55
3:L:419:PRO:HD2	3:L:422:PHE:CZ	2.40	0.55
3:D:142:HIS:CD2	3:D:142:HIS:N	2.75	0.55
3:D:436:ASN:O	3:D:438:LEU:N	2.39	0.55
2:G:955:LEU:HD23	2:G:989:ILE:HG13	1.88	0.55
2:I:782:PRO:HG2	2:I:785:VAL:HG23	1.87	0.55
2:I:850:LEU:HD11	2:I:854:PHE:CE2	2.42	0.55
3:J:384:VAL:HG22	3:J:407:TYR:HB2	1.89	0.55
1:A:354:PHE:HD1	1:A:354:PHE:N	2.04	0.55
1:C:344:LEU:HD13	1:C:402:PHE:HB2	1.88	0.55
3:D:369:LEU:HD13	3:D:390:ASN:OD1	2.07	0.55
1:F:354:PHE:HD1	1:F:354:PHE:N	2.05	0.55
3:J:421:GLU:C	3:J:424:ASN:HB2	2.27	0.55
3:D:143:PRO:HD2	3:D:157:TRP:CH2	2.42	0.55
3:D:512:THR:O	3:D:512:THR:HG23	2.07	0.55
1:E:154:PRO:HG2	1:E:157:TYR:CD1	2.42	0.55
2:H:951:LEU:HD13	2:H:988:PHE:HD2	1.72	0.55
3:K:174:PRO:O	3:K:179:ARG:NH2	2.39	0.55
3:K:415:VAL:H	3:K:436:ASN:HB3	1.72	0.55
1:A:387:ILE:O	1:A:393:GLY:HA3	2.07	0.55
1:F:213:MET:HG3	1:F:309:TYR:CE1	2.42	0.55
1:F:344:LEU:HD13	1:F:402:PHE:HB2	1.89	0.55
2:H:798:LEU:HD12	2:H:838:LEU:HD13	1.89	0.55
3:D:160:GLN:NE2	3:D:430:PHE:HE1	2.05	0.55
3:D:367:ASN:HB2	3:D:369:LEU:HD13	1.88	0.55
2:I:798:LEU:HD12	2:I:838:LEU:HD13	1.87	0.55
2:I:834:ASN:HB2	2:I:835:TYR:CD1	2.42	0.55
3:K:346:ILE:HB	3:K:367:ASN:ND2	2.21	0.55
1:A:354:PHE:N	1:A:354:PHE:CD1	2.73	0.54
3:J:148:ASP:HB3	3:J:149:PRO:O	2.06	0.54
1:A:199:ILE:HG22	1:A:200:GLY:H	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:347:PHE:HD1	3:D:347:PHE:H	1.53	0.54
2:H:834:ASN:HB2	2:H:835:TYR:CD1	2.43	0.54
1:A:191:PHE:CZ	1:A:309:TYR:CD2	2.94	0.54
1:E:348:TYR:CE1	1:E:376:LEU:HD13	2.43	0.54
1:F:354:PHE:HD2	1:F:414:PRO:HB2	1.72	0.54
2:H:800:ASN:ND2	2:H:804:LYS:HG3	2.22	0.54
3:K:443:LEU:O	3:K:447:THR:HG23	2.07	0.54
1:F:154:PRO:HG2	1:F:157:TYR:CE1	2.42	0.54
2:G:953:ILE:HG22	2:G:985:PRO:HB3	1.89	0.54
3:K:424:ASN:ND2	3:K:807:ILE:HG21	2.14	0.54
2:B:826:THR:HG22	2:B:862:GLN:OE1	2.08	0.54
1:E:354:PHE:N	1:E:354:PHE:CD1	2.74	0.54
3:J:420:TRP:CE2	3:J:463:PRO:CD	2.89	0.54
3:L:393:THR:HA	3:L:414:MET:O	2.07	0.54
3:L:418:LEU:HD11	3:L:454:LEU:HD21	1.90	0.54
3:D:457:TYR:CD1	3:D:457:TYR:C	2.80	0.54
3:K:367:ASN:HB2	3:K:369:LEU:HD13	1.90	0.54
3:K:416:THR:O	3:K:438:LEU:HD23	2.07	0.54
2:B:910:ILE:HD11	2:B:988:PHE:HB3	1.88	0.54
2:B:940:PRO:HA	2:B:942:ASN:H	1.73	0.54
1:E:207:ASP:O	1:E:211:GLN:HG2	2.08	0.54
2:I:800:ASN:ND2	2:I:804:LYS:HG3	2.23	0.54
2:I:907:GLU:OE1	2:I:907:GLU:N	2.30	0.54
3:K:156:ILE:HG21	3:K:447:THR:HA	1.88	0.54
3:K:540:LEU:CD2	3:K:815:PRO:HG2	2.38	0.54
3:D:381:ASN:O	3:D:383:ARG:NH1	2.41	0.54
3:K:143:PRO:HD2	3:K:157:TRP:CZ2	2.42	0.54
1:A:354:PHE:HD2	1:A:414:PRO:HB2	1.73	0.54
3:D:420:TRP:O	3:D:422:PHE:O	2.26	0.54
3:D:341:LEU:HB2	3:D:364:LEU:HD23	1.88	0.54
1:F:199:ILE:HG22	1:F:200:GLY:H	1.70	0.54
1:F:354:PHE:N	1:F:354:PHE:CD1	2.75	0.54
3:K:457:TYR:CD1	3:K:457:TYR:C	2.81	0.54
3:K:817:ASP:OD1	3:K:817:ASP:N	2.37	0.53
2:B:956:ASN:OD1	2:B:966:THR:HG23	2.08	0.53
3:D:152:LEU:HD12	3:D:152:LEU:H	1.72	0.53
1:F:376:LEU:HD11	1:F:405:LEU:HD22	1.89	0.53
1:F:387:ILE:O	1:F:393:GLY:HA3	2.07	0.53
3:J:140:LEU:HG	3:J:437:PRO:HB3	1.89	0.53
3:J:252:ASP:O	3:J:256:ASP:HB2	2.08	0.53
3:J:335:LEU:O	3:J:337:HIS:ND1	2.40	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:422:PHE:HB3	3:K:425:LEU:CD2	2.38	0.53
3:K:567:VAL:CG1	3:K:568:PRO:CD	2.84	0.53
3:L:138:ASN:HB3	3:L:141:LEU:HD23	1.90	0.53
3:L:421:GLU:C	3:L:424:ASN:HB2	2.29	0.53
2:B:813:THR:HG22	2:B:814:PRO:HD2	1.91	0.53
1:C:354:PHE:CD1	1:C:354:PHE:N	2.75	0.53
3:D:567:VAL:CG1	3:D:568:PRO:CD	2.84	0.53
1:A:199:ILE:HD13	3:D:178:ALA:HA	1.91	0.53
2:B:800:ASN:ND2	2:B:804:LYS:HG3	2.24	0.53
2:H:971:VAL:O	2:H:974:LYS:HB3	2.08	0.53
2:I:812:LEU:HD21	2:I:820:PHE:HD2	1.73	0.53
3:K:422:PHE:CB	3:K:425:LEU:CG	2.85	0.53
3:J:393:THR:HA	3:J:414:MET:O	2.07	0.53
3:K:346:ILE:H	3:K:367:ASN:HB3	1.73	0.53
3:K:523:TYR:CD1	3:K:523:TYR:N	2.74	0.53
1:A:273:GLU:OE1	1:A:273:GLU:N	2.40	0.53
2:B:834:ASN:HB2	2:B:835:TYR:CD1	2.44	0.53
2:H:953:ILE:HG22	2:H:985:PRO:HB3	1.91	0.53
3:J:420:TRP:NE1	3:J:463:PRO:CD	2.72	0.53
3:D:346:ILE:H	3:D:367:ASN:HB3	1.73	0.53
3:J:446:LEU:O	3:J:450:SER:HA	2.08	0.53
3:L:148:ASP:HB3	3:L:149:PRO:O	2.08	0.53
3:L:163:LEU:HD12	3:L:430:PHE:CE1	2.43	0.53
3:L:252:ASP:O	3:L:256:ASP:HB2	2.08	0.53
1:A:344:LEU:HD21	1:A:376:LEU:HD23	1.91	0.53
3:D:143:PRO:HD2	3:D:157:TRP:CZ2	2.44	0.53
3:D:422:PHE:CB	3:D:425:LEU:CG	2.86	0.53
2:I:867:LEU:HD23	2:I:920:ILE:HG22	1.91	0.53
3:J:397:ALA:HB1	3:J:421:GLU:HG3	1.90	0.53
3:D:335:LEU:O	3:D:337:HIS:ND1	2.42	0.53
3:K:768:PHE:CD2	3:K:771:PHE:HB2	2.44	0.53
1:A:350:ILE:HD11	1:A:422:TYR:CE2	2.44	0.53
1:C:354:PHE:N	1:C:354:PHE:HD1	2.05	0.53
3:D:540:LEU:CD2	3:D:815:PRO:HG2	2.39	0.52
2:I:826:THR:HG22	2:I:862:GLN:OE1	2.09	0.52
3:L:411:PHE:O	3:L:412:ASP:CB	2.57	0.52
3:D:443:LEU:O	3:D:447:THR:HG23	2.09	0.52
2:H:910:ILE:HD11	2:H:988:PHE:HB3	1.89	0.52
1:A:219:PHE:HE1	3:D:356:TYR:CD1	2.27	0.52
1:A:247:ASN:HB3	1:A:275:HIS:CE1	2.44	0.52
3:D:376:ILE:O	3:D:379:LEU:HB2	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:978:LEU:HB3	2:I:982:SER:OG	2.09	0.52
3:J:152:LEU:HD12	3:J:152:LEU:H	1.73	0.52
3:J:344:LEU:O	3:J:346:ILE:HB	2.10	0.52
3:J:419:PRO:O	3:J:420:TRP:HB2	2.09	0.52
3:K:392:LEU:HD12	3:K:413:ASN:ND2	2.24	0.52
2:G:867:LEU:HD23	2:G:920:ILE:HG22	1.92	0.52
3:K:514:CYS:HG	3:K:517:TYR:HD1	1.56	0.52
1:C:350:ILE:HD11	1:C:422:TYR:CE2	2.45	0.52
3:D:173:GLN:O	3:D:176:ILE:HD13	2.10	0.52
3:L:410:PHE:CZ	3:L:433:VAL:HG12	2.43	0.52
3:L:423:GLY:HA2	3:L:455:ILE:HD12	1.91	0.52
2:H:812:LEU:HD23	2:H:846:MET:CE	2.40	0.52
2:H:813:THR:HG22	2:H:814:PRO:HD2	1.92	0.52
3:J:141:LEU:CD1	3:J:437:PRO:HD3	2.40	0.52
3:J:438:LEU:HD13	3:J:443:LEU:HD23	1.92	0.52
1:F:289:LEU:HD23	1:F:318:LEU:HD21	1.92	0.52
1:C:191:PHE:CZ	1:C:309:TYR:CD2	2.97	0.52
1:E:376:LEU:HD11	1:E:405:LEU:HD22	1.91	0.52
2:H:788:LYS:O	2:H:792:VAL:HG23	2.09	0.52
3:J:410:PHE:CD1	3:J:410:PHE:N	2.77	0.52
3:K:335:LEU:O	3:K:337:HIS:ND1	2.43	0.52
1:A:191:PHE:HZ	1:A:309:TYR:HD2	1.55	0.52
3:K:451:VAL:HG12	3:K:452:THR:N	2.25	0.52
3:L:407:TYR:CD1	3:L:407:TYR:N	2.78	0.52
3:K:422:PHE:CA	3:K:424:ASN:H	2.23	0.52
1:C:376:LEU:HD11	1:C:405:LEU:HD22	1.91	0.51
3:K:549:SER:HB3	3:K:552:LEU:CD2	2.40	0.51
1:A:376:LEU:HD11	1:A:405:LEU:HD22	1.91	0.51
3:D:447:THR:O	3:D:448:GLU:CD	2.49	0.51
3:D:559:SER:O	3:D:563:GLU:HG2	2.11	0.51
1:E:199:ILE:HG22	1:E:200:GLY:H	1.73	0.51
1:F:354:PHE:O	1:F:355:LYS:CB	2.58	0.51
2:I:911:GLU:O	2:I:915:GLU:HG2	2.10	0.51
3:J:403:PHE:HD1	3:J:404:GLN:N	2.09	0.51
3:J:418:LEU:HD11	3:J:454:LEU:HD21	1.92	0.51
3:J:422:PHE:HB3	3:J:425:LEU:CG	2.38	0.51
3:K:145:HIS:O	3:K:145:HIS:ND1	2.44	0.51
2:B:971:VAL:O	2:B:974:LYS:HB3	2.10	0.51
3:D:418:LEU:HB3	3:D:422:PHE:CE1	2.37	0.51
3:D:451:VAL:HG12	3:D:452:THR:N	2.26	0.51
3:K:422:PHE:HD2	3:K:425:LEU:HD21	1.74	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:150:SER:CA	3:L:152:LEU:HD12	2.33	0.51
3:L:396:PRO:C	3:L:397:ALA:O	2.40	0.51
3:L:417:THR:HG23	3:L:442:PHE:HE2	1.73	0.51
3:L:446:LEU:O	3:L:450:SER:HA	2.09	0.51
1:A:348:TYR:CE1	1:A:376:LEU:HD13	2.46	0.51
2:B:812:LEU:HD21	2:B:820:PHE:HD2	1.75	0.51
1:E:193:GLY:C	1:E:195:LEU:HD23	2.30	0.51
3:J:411:PHE:O	3:J:412:ASP:CB	2.59	0.51
3:K:434:GLU:OE1	3:K:435:GLY:HA3	2.11	0.51
3:L:428:LEU:HD21	3:L:431:LEU:HB2	1.91	0.51
1:C:154:PRO:HG2	1:C:157:TYR:CD1	2.45	0.51
1:C:387:ILE:O	1:C:393:GLY:HA3	2.10	0.51
3:L:141:LEU:CD1	3:L:437:PRO:HD3	2.41	0.51
3:L:422:PHE:HB3	3:L:425:LEU:CG	2.38	0.51
3:L:403:PHE:HD1	3:L:404:GLN:N	2.09	0.51
2:B:812:LEU:HD23	2:B:846:MET:CE	2.41	0.51
3:K:341:LEU:HB2	3:K:364:LEU:HD23	1.91	0.51
2:H:909:LEU:HD12	2:H:951:LEU:HD23	1.92	0.51
2:B:798:LEU:HD12	2:B:838:LEU:HD13	1.93	0.51
1:C:194:THR:HG23	1:C:194:THR:O	2.11	0.51
3:D:145:HIS:O	3:D:145:HIS:ND1	2.44	0.51
3:D:421:GLU:O	3:D:424:ASN:HB2	2.11	0.51
3:K:418:LEU:HB3	3:K:422:PHE:CE1	2.38	0.51
3:K:447:THR:O	3:K:448:GLU:CD	2.50	0.51
3:L:410:PHE:HE1	3:L:431:LEU:HD11	1.76	0.51
3:L:420:TRP:CE2	3:L:463:PRO:CD	2.94	0.51
1:A:391:THR:O	1:A:394:GLN:HB2	2.11	0.51
2:I:953:ILE:HG22	2:I:985:PRO:HB3	1.92	0.51
3:J:407:TYR:N	3:J:407:TYR:CD1	2.79	0.51
3:J:461:ASN:N	3:J:461:ASN:OD1	2.42	0.51
1:C:344:LEU:HD21	1:C:376:LEU:HD23	1.93	0.50
3:L:419:PRO:CD	3:L:422:PHE:CE1	2.93	0.50
3:D:526:THR:HB	3:D:810:PRO:O	2.11	0.50
3:L:410:PHE:CD1	3:L:410:PHE:N	2.78	0.50
1:C:252:PRO:HB3	1:C:257:MET:CE	2.41	0.50
3:D:174:PRO:O	3:D:179:ARG:NH2	2.45	0.50
1:E:273:GLU:N	1:E:273:GLU:OE1	2.43	0.50
3:J:423:GLY:HA2	3:J:455:ILE:HD12	1.93	0.50
3:L:152:LEU:HD12	3:L:152:LEU:H	1.76	0.50
1:C:182:TYR:CZ	1:C:237:PRO:HD3	2.46	0.50
3:D:549:SER:HB3	3:D:552:LEU:CD2	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:154:PRO:HG2	1:E:157:TYR:CE1	2.46	0.50
3:J:163:LEU:HD12	3:J:430:PHE:CE1	2.46	0.50
3:K:451:VAL:O	3:K:454:LEU:N	2.44	0.50
3:L:461:ASN:N	3:L:461:ASN:OD1	2.44	0.50
2:B:951:LEU:HD13	2:B:988:PHE:HD2	1.76	0.50
3:D:422:PHE:CD2	3:D:425:LEU:HD21	2.47	0.50
3:D:800:PRO:HA	3:D:803:VAL:HG22	1.93	0.50
1:E:199:ILE:HD13	3:L:178:ALA:HA	1.93	0.50
2:G:812:LEU:HD21	2:G:820:PHE:HD2	1.76	0.50
2:H:826:THR:HG22	2:H:862:GLN:OE1	2.12	0.50
3:J:444:LYS:HE3	3:J:448:GLU:OE2	2.10	0.50
1:A:219:PHE:CE2	3:D:353:ILE:HG22	2.46	0.50
1:C:199:ILE:HD13	3:K:178:ALA:HA	1.94	0.50
1:C:355:LYS:HB2	1:C:355:LYS:NZ	2.26	0.50
1:E:304:THR:HB	1:E:307:ALA:HB2	1.94	0.50
1:E:354:PHE:O	1:E:355:LYS:CB	2.59	0.50
3:K:160:GLN:NE2	3:K:430:PHE:HE1	2.09	0.50
3:L:335:LEU:O	3:L:337:HIS:ND1	2.44	0.50
1:C:219:PHE:HE1	3:K:356:TYR:CD1	2.30	0.50
2:G:911:GLU:O	2:G:915:GLU:HG2	2.12	0.50
2:I:955:LEU:HD23	2:I:989:ILE:HG13	1.93	0.50
3:K:559:SER:O	3:K:563:GLU:HG2	2.12	0.50
3:L:397:ALA:C	3:L:399:LEU:H	2.15	0.50
3:D:817:ASP:OD1	3:D:817:ASP:N	2.39	0.50
1:F:151:PHE:C	1:F:151:PHE:HD1	2.14	0.50
1:F:273:GLU:OE1	1:F:273:GLU:N	2.44	0.50
3:L:163:LEU:HD12	3:L:430:PHE:CZ	2.46	0.50
3:L:422:PHE:HB2	3:L:425:LEU:CD1	2.42	0.50
1:C:151:PHE:C	1:C:151:PHE:HD1	2.15	0.49
1:C:207:ASP:O	1:C:211:GLN:HG2	2.11	0.49
1:F:191:PHE:HZ	1:F:309:TYR:CD2	2.29	0.49
3:L:344:LEU:O	3:L:346:ILE:HB	2.12	0.49
1:F:298:ASP:OD1	1:F:298:ASP:N	2.34	0.49
3:K:428:LEU:HB3	3:K:455:ILE:CD1	2.41	0.49
3:K:800:PRO:HA	3:K:803:VAL:HG22	1.92	0.49
1:E:298:ASP:OD1	1:E:298:ASP:N	2.35	0.49
1:E:387:ILE:O	1:E:393:GLY:HA3	2.12	0.49
3:K:421:GLU:O	3:K:424:ASN:HB2	2.12	0.49
3:K:526:THR:HB	3:K:810:PRO:O	2.12	0.49
2:B:956:ASN:ND2	2:B:966:THR:HG23	2.26	0.49
1:C:298:ASP:OD1	1:C:298:ASP:N	2.36	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:350:ILE:HD11	1:E:422:TYR:CE2	2.47	0.49
2:H:867:LEU:HD23	2:H:920:ILE:HG22	1.95	0.49
3:K:173:GLN:O	3:K:176:ILE:HD13	2.12	0.49
3:K:459:ARG:NE	3:K:460:ASP:OD1	2.44	0.49
3:L:374:ALA:CB	3:L:398:GLU:OE2	2.59	0.49
3:J:417:THR:HG23	3:J:442:PHE:HE2	1.77	0.49
3:J:442:PHE:CE1	3:J:458:LEU:HD21	2.42	0.49
3:L:177:TYR:CD2	3:L:363:TYR:CE1	3.00	0.49
3:L:342:SER:HA	3:L:365:ASN:O	2.13	0.49
3:L:397:ALA:HB1	3:L:421:GLU:HG3	1.93	0.49
2:B:796:VAL:HG13	2:B:838:LEU:HD21	1.95	0.49
1:C:163:VAL:HG12	1:C:280:ILE:HD11	1.94	0.49
3:D:434:GLU:OE1	3:D:435:GLY:HA3	2.13	0.49
2:G:826:THR:HG22	2:G:862:GLN:OE1	2.12	0.49
2:G:867:LEU:HD13	2:G:908:MET:HE1	1.94	0.49
3:J:343:ASN:HA	3:J:366:GLY:O	2.12	0.49
3:L:347:PHE:CD1	3:L:368:SER:HB2	2.44	0.49
1:C:191:PHE:HZ	1:C:309:TYR:HD2	1.58	0.49
3:D:519:THR:HG23	3:D:522:MET:CE	2.43	0.49
1:F:350:ILE:HD11	1:F:422:TYR:CE2	2.47	0.49
3:K:519:THR:HG23	3:K:522:MET:CE	2.43	0.49
3:L:388:SER:HB3	3:L:389:HIS:CD2	2.48	0.49
1:C:154:PRO:HG2	1:C:157:TYR:CE1	2.48	0.49
3:K:441:GLN:O	3:K:445:ILE:HG12	2.13	0.49
3:D:156:ILE:HG21	3:D:447:THR:HA	1.94	0.49
3:D:446:LEU:HA	3:D:450:SER:O	2.13	0.49
1:E:191:PHE:HZ	1:E:309:TYR:CD2	2.30	0.49
2:H:796:VAL:HG13	2:H:838:LEU:HD21	1.94	0.49
2:H:940:PRO:HA	2:H:942:ASN:N	2.28	0.49
2:H:981:LYS:HE2	2:H:981:LYS:HA	1.95	0.49
3:J:177:TYR:CD2	3:J:363:TYR:CE1	3.00	0.49
3:K:177:TYR:CD2	3:K:363:TYR:CE1	3.01	0.49
3:K:376:ILE:O	3:K:379:LEU:HB2	2.13	0.49
3:D:397:ALA:C	3:D:399:LEU:N	2.63	0.48
3:D:423:GLY:C	3:D:425:LEU:N	2.65	0.48
2:G:835:TYR:CD1	2:G:835:TYR:N	2.81	0.48
3:L:410:PHE:O	3:L:410:PHE:CD2	2.66	0.48
3:L:444:LYS:HE3	3:L:448:GLU:OE2	2.13	0.48
1:C:151:PHE:HD1	1:C:152:LEU:N	2.10	0.48
1:C:380:LEU:HD23	1:C:380:LEU:HA	1.66	0.48
1:E:193:GLY:O	1:E:195:LEU:HG	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:191:PHE:CZ	1:F:309:TYR:CD2	2.92	0.48
2:H:956:ASN:ND2	2:H:966:THR:HG23	2.28	0.48
2:I:813:THR:HG22	2:I:814:PRO:HD2	1.94	0.48
3:J:374:ALA:CB	3:J:398:GLU:OE2	2.60	0.48
3:J:420:TRP:CD1	3:J:463:PRO:HD2	2.48	0.48
1:C:354:PHE:O	1:C:355:LYS:HG2	2.14	0.48
3:D:422:PHE:HB3	3:D:425:LEU:CD2	2.43	0.48
1:E:307:ALA:HB1	1:E:311:LEU:HG	1.95	0.48
2:B:867:LEU:HD23	2:B:920:ILE:HG22	1.96	0.48
2:G:791:PHE:HE1	2:G:795:ASN:ND2	2.11	0.48
3:L:161:LEU:HD23	3:L:434:GLU:HG3	1.95	0.48
3:J:163:LEU:HD12	3:J:430:PHE:CZ	2.48	0.48
1:A:151:PHE:HD1	1:A:152:LEU:N	2.10	0.48
1:A:307:ALA:HB1	1:A:311:LEU:HG	1.96	0.48
3:D:428:LEU:HB3	3:D:455:ILE:CD1	2.41	0.48
2:B:981:LYS:HE2	2:B:981:LYS:HA	1.96	0.48
1:C:219:PHE:HE1	3:K:356:TYR:CE1	2.32	0.48
1:F:151:PHE:HD1	1:F:152:LEU:N	2.12	0.48
1:F:348:TYR:CE1	1:F:376:LEU:HD13	2.49	0.48
3:J:142:HIS:ND1	3:J:434:GLU:OE2	2.46	0.48
3:K:410:PHE:CG	3:K:410:PHE:O	2.66	0.48
3:K:804:SER:O	3:K:805:LYS:HB2	2.14	0.48
1:F:168:LEU:HD13	1:F:280:ILE:HD12	1.95	0.48
2:I:971:VAL:O	2:I:974:LYS:HB3	2.13	0.48
3:J:347:PHE:CD1	3:J:368:SER:HB2	2.45	0.48
1:A:151:PHE:C	1:A:151:PHE:HD1	2.18	0.48
1:A:191:PHE:HD1	1:A:191:PHE:H	1.62	0.48
1:A:304:THR:HB	1:A:307:ALA:HB2	1.95	0.48
2:B:909:LEU:HD12	2:B:951:LEU:HD23	1.96	0.48
2:B:978:LEU:HB3	2:B:982:SER:OG	2.14	0.48
1:E:151:PHE:C	1:E:151:PHE:HD1	2.16	0.48
3:K:769:THR:O	3:K:818:HIS:HA	2.14	0.48
1:C:304:THR:HB	1:C:307:ALA:HB2	1.95	0.47
3:K:410:PHE:HE1	3:K:431:LEU:HD11	1.78	0.47
3:K:425:LEU:O	3:K:455:ILE:HD13	2.14	0.47
1:A:163:VAL:HG12	1:A:280:ILE:HD11	1.96	0.47
1:A:194:THR:HG23	1:A:194:THR:O	2.14	0.47
1:A:354:PHE:O	1:A:355:LYS:CB	2.61	0.47
3:D:425:LEU:O	3:D:455:ILE:HD13	2.14	0.47
2:G:981:LYS:HA	2:G:981:LYS:HE2	1.96	0.47
3:J:422:PHE:HB2	3:J:425:LEU:CG	2.40	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:258:SER:O	1:F:259:THR:C	2.53	0.47
1:F:304:THR:HB	1:F:307:ALA:HB2	1.96	0.47
2:G:788:LYS:O	2:G:792:VAL:HG23	2.13	0.47
2:G:971:VAL:O	2:G:974:LYS:HB3	2.13	0.47
2:H:791:PHE:HE1	2:H:795:ASN:ND2	2.12	0.47
3:K:397:ALA:C	3:K:399:LEU:N	2.65	0.47
1:C:247:ASN:HB3	1:C:275:HIS:CE1	2.49	0.47
1:C:273:GLU:N	1:C:273:GLU:OE1	2.47	0.47
3:D:397:ALA:HA	3:D:421:GLU:HG3	1.95	0.47
1:E:151:PHE:HD1	1:E:152:LEU:N	2.12	0.47
3:D:346:ILE:O	3:D:369:LEU:HD12	2.15	0.47
3:D:441:GLN:O	3:D:445:ILE:HG12	2.15	0.47
1:F:182:TYR:CZ	1:F:237:PRO:HD3	2.50	0.47
1:F:344:LEU:HD21	1:F:376:LEU:HD23	1.95	0.47
1:F:346:LEU:HD23	1:F:346:LEU:O	2.13	0.47
2:I:901:LYS:HG2	2:I:902:ASN:N	2.29	0.47
3:K:423:GLY:C	3:K:425:LEU:N	2.67	0.47
3:L:372:LEU:HD12	3:L:373:PRO:HD2	1.95	0.47
2:B:809:LYS:HG3	2:B:846:MET:SD	2.54	0.47
1:C:182:TYR:CE2	1:C:237:PRO:HD3	2.50	0.47
3:D:451:VAL:O	3:D:454:LEU:N	2.47	0.47
2:H:764:LEU:HD12	2:H:864:PHE:CD1	2.50	0.47
3:J:413:ASN:O	3:J:436:ASN:HB3	2.14	0.47
3:K:186:TYR:CD1	3:K:186:TYR:C	2.88	0.47
3:K:536:ARG:O	3:K:540:LEU:HG	2.15	0.47
1:C:193:GLY:C	1:C:195:LEU:HD23	2.35	0.47
3:D:769:THR:O	3:D:818:HIS:HA	2.14	0.47
1:E:182:TYR:CZ	1:E:237:PRO:HD3	2.50	0.47
1:F:225:LEU:C	1:F:225:LEU:HD23	2.35	0.47
2:G:809:LYS:HG3	2:G:846:MET:SD	2.55	0.47
2:H:834:ASN:HB2	2:H:835:TYR:CE1	2.49	0.47
2:I:788:LYS:O	2:I:792:VAL:HG23	2.14	0.47
3:J:358:PHE:N	3:J:358:PHE:CD1	2.82	0.47
3:J:372:LEU:HD12	3:J:373:PRO:HD2	1.96	0.47
3:J:397:ALA:C	3:J:399:LEU:N	2.66	0.47
3:J:410:PHE:CZ	3:J:433:VAL:HG12	2.48	0.47
3:J:422:PHE:CB	3:J:425:LEU:CG	2.83	0.47
3:K:143:PRO:HG3	3:K:443:LEU:HD13	1.97	0.47
3:L:410:PHE:O	3:L:410:PHE:CG	2.68	0.47
3:L:413:ASN:O	3:L:436:ASN:HB3	2.14	0.47
1:C:179:VAL:HG23	1:C:294:LEU:HD23	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:436:ASN:OD1	3:D:436:ASN:N	2.48	0.47
3:D:579:PHE:HZ	3:D:598:GLY:HA3	1.79	0.47
1:A:154:PRO:HG2	1:A:157:TYR:CE1	2.50	0.47
1:A:191:PHE:HZ	1:A:309:TYR:CD2	2.32	0.47
2:B:940:PRO:HA	2:B:942:ASN:N	2.29	0.47
2:G:796:VAL:HG13	2:G:838:LEU:HD21	1.97	0.47
3:K:152:LEU:HD12	3:K:152:LEU:H	1.79	0.47
3:K:244:LYS:CB	3:K:247:LEU:HB2	2.45	0.47
1:A:202:PHE:HB2	1:A:203:ARG:H	1.48	0.47
3:D:173:GLN:CB	3:D:179:ARG:HH12	2.28	0.47
3:D:177:TYR:CD2	3:D:363:TYR:CE1	3.03	0.47
2:I:940:PRO:HA	2:I:942:ASN:H	1.79	0.47
3:L:438:LEU:HD13	3:L:443:LEU:HD23	1.97	0.47
1:C:219:PHE:CE1	3:K:356:TYR:CE1	3.03	0.46
1:E:191:PHE:CZ	1:E:309:TYR:CD2	2.94	0.46
2:I:981:LYS:HE2	2:I:981:LYS:HA	1.96	0.46
3:K:163:LEU:HD11	3:K:249:GLU:CA	2.40	0.46
3:D:339:LEU:HB2	3:D:359:LEU:HD11	1.97	0.46
1:F:346:LEU:HD23	1:F:346:LEU:C	2.36	0.46
3:J:341:LEU:O	3:J:344:LEU:HD11	2.15	0.46
3:J:419:PRO:CD	3:J:422:PHE:HE1	2.28	0.46
3:L:425:LEU:CD1	3:L:428:LEU:HD22	2.45	0.46
1:A:219:PHE:CD2	3:D:353:ILE:HG22	2.51	0.46
3:D:151:LEU:HB3	3:D:157:TRP:HB3	1.97	0.46
3:D:186:TYR:CD1	3:D:186:TYR:C	2.88	0.46
3:D:410:PHE:HE1	3:D:431:LEU:HD11	1.79	0.46
3:D:410:PHE:O	3:D:410:PHE:CG	2.68	0.46
3:D:452:THR:HA	3:D:455:ILE:HB	1.98	0.46
3:D:550:ASP:O	3:D:603:PHE:HA	2.16	0.46
3:K:446:LEU:HA	3:K:450:SER:O	2.16	0.46
3:D:384:VAL:HA	3:D:407:TYR:O	2.15	0.46
2:H:956:ASN:OD1	2:H:966:THR:HG23	2.16	0.46
2:I:956:ASN:ND2	2:I:966:THR:HG23	2.29	0.46
3:J:364:LEU:HD23	3:J:364:LEU:HA	1.76	0.46
3:J:422:PHE:CD1	3:J:422:PHE:C	2.88	0.46
1:A:219:PHE:CE1	3:D:353:ILE:HA	2.51	0.46
1:A:380:LEU:HA	1:A:380:LEU:HD23	1.69	0.46
1:C:391:THR:O	1:C:394:GLN:HB2	2.16	0.46
3:D:465:ILE:HA	3:D:466:PRO:HD2	1.68	0.46
1:E:344:LEU:HD13	1:E:402:PHE:HB2	1.97	0.46
2:G:978:LEU:HB3	2:G:982:SER:OG	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:812:LEU:HD23	2:H:846:MET:HE1	1.98	0.46
2:H:880:LEU:CD2	2:H:920:ILE:HG23	2.45	0.46
3:J:161:LEU:HD23	3:J:434:GLU:HG3	1.98	0.46
3:K:372:LEU:HB3	3:K:396:PRO:HG3	1.97	0.46
3:L:142:HIS:ND1	3:L:434:GLU:OE2	2.48	0.46
1:A:252:PRO:HB3	1:A:257:MET:CE	2.45	0.46
3:D:434:GLU:HA	3:D:435:GLY:HA2	1.54	0.46
2:I:835:TYR:CD1	2:I:835:TYR:N	2.83	0.46
3:K:151:LEU:HB3	3:K:157:TRP:HB3	1.98	0.46
2:B:835:TYR:CD1	2:B:835:TYR:N	2.84	0.46
2:G:940:PRO:HA	2:G:942:ASN:H	1.81	0.46
2:I:764:LEU:HD12	2:I:864:PHE:CD1	2.51	0.46
3:K:346:ILE:HD12	3:K:367:ASN:ND2	2.30	0.46
3:K:431:LEU:O	3:K:431:LEU:HG	2.16	0.46
2:B:764:LEU:HD12	2:B:864:PHE:CD1	2.51	0.46
1:C:213:MET:HG3	1:C:309:TYR:CE1	2.50	0.46
3:J:388:SER:HB3	3:J:389:HIS:CD2	2.51	0.46
3:D:383:ARG:HA	3:D:405:LEU:HA	1.97	0.46
1:F:184:HIS:O	1:F:229:LEU:HA	2.16	0.46
3:J:138:ASN:HB3	3:J:141:LEU:HD23	1.97	0.46
3:K:397:ALA:HA	3:K:421:GLU:HG3	1.98	0.46
3:D:143:PRO:HG3	3:D:443:LEU:HD13	1.98	0.45
2:I:834:ASN:HB2	2:I:835:TYR:CE1	2.51	0.45
3:K:356:TYR:CD2	3:K:358:PHE:HE1	2.33	0.45
3:L:422:PHE:CD1	3:L:422:PHE:C	2.89	0.45
2:B:788:LYS:O	2:B:792:VAL:HG23	2.16	0.45
2:B:834:ASN:HB2	2:B:835:TYR:CE1	2.51	0.45
1:A:344:LEU:HD13	1:A:402:PHE:HB2	1.97	0.45
1:C:380:LEU:HD22	1:C:404:GLN:HG2	1.98	0.45
3:D:372:LEU:HB3	3:D:396:PRO:HG3	1.98	0.45
1:E:193:GLY:C	1:E:195:LEU:CD2	2.85	0.45
1:E:219:PHE:CZ	3:L:356:TYR:CE2	3.04	0.45
1:E:344:LEU:HD21	1:E:376:LEU:HD23	1.97	0.45
2:H:911:GLU:O	2:H:915:GLU:HG2	2.15	0.45
3:J:379:LEU:HD23	3:J:379:LEU:HA	1.74	0.45
3:K:434:GLU:HA	3:K:435:GLY:HA2	1.55	0.45
3:L:376:ILE:O	3:L:379:LEU:HB2	2.16	0.45
1:C:165:LYS:NZ	1:C:165:LYS:HB3	2.30	0.45
3:D:405:LEU:HD13	3:D:408:PHE:HB2	1.98	0.45
1:E:380:LEU:HD22	1:E:404:GLN:HG2	1.98	0.45
3:J:345:GLN:CD	3:J:345:GLN:H	2.19	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:372:LEU:HA	3:J:373:PRO:HD2	1.87	0.45
3:L:167:SER:O	3:L:170:SER:HB2	2.17	0.45
3:L:383:ARG:HG2	3:L:406:LYS:HG3	1.99	0.45
3:D:799:ASP:O	3:D:802:TYR:HB3	2.17	0.45
1:F:307:ALA:HB1	1:F:311:LEU:HG	1.99	0.45
2:H:921:VAL:O	2:H:924:PHE:HB3	2.17	0.45
2:H:978:LEU:HB3	2:H:982:SER:OG	2.17	0.45
3:K:396:PRO:C	3:K:397:ALA:O	2.53	0.45
1:A:154:PRO:HG2	1:A:157:TYR:CD1	2.51	0.45
1:C:168:LEU:HD13	1:C:280:ILE:HD12	1.99	0.45
3:D:579:PHE:O	3:D:579:PHE:CD1	2.70	0.45
1:F:402:PHE:CD1	1:F:402:PHE:C	2.90	0.45
2:G:813:THR:HG22	2:G:814:PRO:HD2	1.99	0.45
2:G:951:LEU:HD13	2:G:988:PHE:HD2	1.82	0.45
2:I:791:PHE:HE1	2:I:795:ASN:ND2	2.14	0.45
2:I:951:LEU:HD13	2:I:988:PHE:HD2	1.82	0.45
3:J:163:LEU:HD23	3:J:163:LEU:HA	1.81	0.45
3:J:375:GLU:C	3:J:377:LYS:N	2.69	0.45
3:K:452:THR:HA	3:K:455:ILE:HB	1.99	0.45
3:L:420:TRP:NE1	3:L:463:PRO:CD	2.80	0.45
1:A:201:THR:O	1:A:202:PHE:CD2	2.70	0.45
1:C:354:PHE:CE2	1:C:415:ASN:ND2	2.85	0.45
2:H:835:TYR:CD1	2:H:835:TYR:N	2.84	0.45
2:H:929:LEU:HD23	2:H:929:LEU:HA	1.61	0.45
2:I:796:VAL:HG13	2:I:838:LEU:HD21	1.99	0.45
3:K:766:LEU:HD12	3:K:766:LEU:HA	1.73	0.45
1:A:179:VAL:HG23	1:A:294:LEU:HD23	1.99	0.45
2:B:791:PHE:HE1	2:B:795:ASN:ND2	2.15	0.45
2:G:921:VAL:O	2:G:925:VAL:HG23	2.17	0.45
3:J:342:SER:HA	3:J:365:ASN:O	2.17	0.45
3:K:384:VAL:HA	3:K:407:TYR:O	2.16	0.45
2:B:812:LEU:HD23	2:B:846:MET:HE1	1.99	0.45
1:C:348:TYR:CE1	1:C:376:LEU:HD13	2.52	0.45
1:E:258:SER:O	1:E:259:THR:C	2.55	0.45
1:E:263:GLU:OE1	1:E:263:GLU:HA	2.16	0.45
2:G:812:LEU:HD23	2:G:846:MET:CE	2.47	0.45
2:G:907:GLU:OE1	2:G:907:GLU:N	2.35	0.45
3:L:345:GLN:H	3:L:345:GLN:CD	2.19	0.45
1:C:202:PHE:O	1:C:203:ARG:HG3	2.17	0.45
3:D:431:LEU:O	3:D:431:LEU:HG	2.17	0.45
1:F:249:GLU:HA	1:F:275:HIS:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:180:GLN:OE1	3:L:244:LYS:HA	2.17	0.45
1:C:201:THR:O	1:C:202:PHE:CD2	2.70	0.44
1:C:307:ALA:HB1	1:C:311:LEU:HG	1.99	0.44
2:I:792:VAL:HG11	2:I:808:LEU:HB2	1.97	0.44
3:L:464:GLU:O	3:L:465:ILE:CB	2.65	0.44
2:B:837:ASP:O	2:B:840:SER:HB3	2.17	0.44
3:D:424:ASN:ND2	3:D:807:ILE:CG2	2.73	0.44
3:J:415:VAL:H	3:J:436:ASN:CB	2.30	0.44
3:L:379:LEU:HD23	3:L:379:LEU:HA	1.77	0.44
3:J:387:LEU:HD13	3:J:392:LEU:HD11	1.98	0.44
3:J:425:LEU:CD1	3:J:428:LEU:HD22	2.47	0.44
3:L:358:PHE:CD1	3:L:358:PHE:N	2.85	0.44
1:C:301:THR:HG23	1:C:340:ASN:OD1	2.17	0.44
3:D:422:PHE:HD2	3:D:425:LEU:HD21	1.82	0.44
3:D:444:LYS:HB3	2:H:963:LEU:CD1	2.46	0.44
1:E:163:VAL:HG12	1:E:280:ILE:HD11	1.97	0.44
1:A:256:ILE:HG12	3:D:349:ILE:HA	2.00	0.44
1:C:168:LEU:HD22	1:C:280:ILE:HG23	1.99	0.44
1:C:191:PHE:HZ	1:C:309:TYR:CD2	2.35	0.44
1:C:258:SER:O	1:C:260:GLU:N	2.50	0.44
1:F:391:THR:O	1:F:394:GLN:HB2	2.18	0.44
2:I:929:LEU:HA	2:I:929:LEU:HD23	1.59	0.44
3:J:361:ARG:O	3:J:384:VAL:O	2.35	0.44
3:K:339:LEU:HB2	3:K:359:LEU:HD11	2.00	0.44
3:K:383:ARG:HA	3:K:405:LEU:HA	1.98	0.44
3:L:361:ARG:O	3:L:384:VAL:O	2.35	0.44
3:L:462:ARG:HA	3:L:463:PRO:HD3	1.67	0.44
1:A:249:GLU:HA	1:A:275:HIS:O	2.18	0.44
1:A:380:LEU:HD22	1:A:404:GLN:HG2	2.00	0.44
1:F:199:ILE:HG22	1:F:200:GLY:N	2.32	0.44
2:G:901:LYS:HG2	2:G:902:ASN:N	2.33	0.44
3:J:176:ILE:HD11	3:J:343:ASN:ND2	2.32	0.44
3:J:392:LEU:O	3:J:413:ASN:HB3	2.18	0.44
3:J:418:LEU:CD1	3:J:454:LEU:HD21	2.47	0.44
3:L:375:GLU:CD	3:L:375:GLU:H	2.20	0.44
3:D:354:PHE:HE2	3:D:373:PRO:HG2	1.80	0.44
2:I:867:LEU:HD13	2:I:908:MET:HE1	1.99	0.44
3:L:363:TYR:HE1	3:L:384:VAL:HG11	1.82	0.44
3:D:514:CYS:HG	3:D:517:TYR:HD1	1.66	0.44
3:D:810:PRO:HB3	3:D:816:SER:N	2.32	0.44
3:J:445:ILE:CD1	3:J:457:TYR:CD2	3.01	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:173:GLN:CB	3:K:179:ARG:HH12	2.31	0.44
3:K:346:ILE:O	3:K:369:LEU:HD12	2.18	0.44
2:B:929:LEU:HD23	2:B:929:LEU:HA	1.65	0.44
1:C:336:GLN:HB3	2:H:937:ILE:HD11	1.99	0.44
3:D:441:GLN:HA	3:D:444:LYS:HD2	2.00	0.44
3:D:555:GLN:C	3:D:599:CYS:SG	2.96	0.44
2:I:812:LEU:HD23	2:I:846:MET:CE	2.48	0.44
3:J:394:SER:O	3:J:395:LEU:HD23	2.17	0.44
3:K:544:ILE:HG23	3:K:552:LEU:CD1	2.47	0.44
3:D:768:PHE:HA	3:D:778:VAL:HG22	2.00	0.43
1:E:168:LEU:HD13	1:E:280:ILE:HD12	1.99	0.43
1:E:391:THR:O	1:E:394:GLN:HB2	2.18	0.43
3:K:177:TYR:HE1	3:K:365:ASN:HD21	1.65	0.43
3:L:388:SER:CB	3:L:389:HIS:CD2	3.01	0.43
1:A:193:GLY:O	1:A:195:LEU:HG	2.18	0.43
2:B:792:VAL:HG11	2:B:808:LEU:HB2	2.00	0.43
1:E:219:PHE:HE2	3:L:339:LEU:HD11	1.83	0.43
1:F:185:VAL:HG23	1:F:229:LEU:HD12	2.00	0.43
2:I:809:LYS:HG3	2:I:846:MET:SD	2.58	0.43
3:K:450:SER:OG	3:K:451:VAL:N	2.50	0.43
3:L:346:ILE:HD13	3:L:346:ILE:HG21	1.55	0.43
3:L:407:TYR:N	3:L:407:TYR:HD1	2.16	0.43
3:D:152:LEU:HD12	3:D:152:LEU:N	2.33	0.43
3:D:160:GLN:NE2	3:D:430:PHE:CZ	2.85	0.43
3:D:392:LEU:CB	3:D:413:ASN:HD22	2.23	0.43
3:K:420:TRP:C	3:K:422:PHE:O	2.57	0.43
3:K:551:LEU:HD21	3:K:601:ILE:HG23	2.00	0.43
1:C:199:ILE:HG22	1:C:200:GLY:N	2.32	0.43
1:C:386:SER:O	1:C:389:THR:HG23	2.18	0.43
3:D:389:HIS:HA	3:D:412:ASP:HB3	2.00	0.43
3:D:441:GLN:O	3:D:444:LYS:HB2	2.18	0.43
3:D:544:ILE:HG23	3:D:552:LEU:CD1	2.48	0.43
2:H:880:LEU:HD22	2:H:920:ILE:HG23	1.99	0.43
3:J:343:ASN:OD1	3:J:366:GLY:HA3	2.17	0.43
3:J:379:LEU:HB3	3:J:382:LEU:HD13	2.00	0.43
3:J:420:TRP:CZ2	3:J:463:PRO:HD3	2.52	0.43
3:K:436:ASN:OD1	3:K:436:ASN:N	2.52	0.43
3:K:441:GLN:HA	3:K:444:LYS:HD2	2.00	0.43
3:L:375:GLU:OE1	3:L:375:GLU:N	2.52	0.43
3:D:356:TYR:CD2	3:D:358:PHE:HE1	2.36	0.43
3:D:369:LEU:HD12	3:D:369:LEU:N	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:766:LEU:HD12	3:D:766:LEU:HA	1.74	0.43
2:G:929:LEU:HA	2:G:929:LEU:HD23	1.55	0.43
3:J:341:LEU:O	3:J:344:LEU:CD1	2.67	0.43
3:K:254:LEU:HD23	3:K:254:LEU:HA	1.70	0.43
3:K:766:LEU:HD12	3:K:767:PRO:CD	2.48	0.43
3:L:345:GLN:N	3:L:345:GLN:CD	2.71	0.43
1:A:165:LYS:NZ	1:A:165:LYS:HB3	2.33	0.43
1:E:332:TRP:CZ2	1:E:336:GLN:HG3	2.54	0.43
1:C:249:GLU:HA	1:C:275:HIS:O	2.19	0.43
3:D:163:LEU:HD23	3:D:163:LEU:HA	1.78	0.43
1:E:346:LEU:HD23	1:E:346:LEU:O	2.18	0.43
2:I:813:THR:HG22	2:I:814:PRO:CD	2.49	0.43
3:J:180:GLN:OE1	3:J:244:LYS:HA	2.19	0.43
3:J:345:GLN:N	3:J:345:GLN:CD	2.72	0.43
3:K:445:ILE:HG13	3:K:457:TYR:HD2	1.84	0.43
3:L:394:SER:O	3:L:395:LEU:HD23	2.18	0.43
1:E:247:ASN:HB3	1:E:275:HIS:CE1	2.53	0.43
1:E:289:LEU:HD23	1:E:318:LEU:HD21	2.01	0.43
1:F:193:GLY:C	1:F:195:LEU:CD2	2.87	0.43
2:I:812:LEU:HD23	2:I:846:MET:HE2	1.99	0.43
3:J:410:PHE:HE1	3:J:431:LEU:HD11	1.84	0.43
3:K:392:LEU:CB	3:K:413:ASN:HD22	2.24	0.43
3:L:387:LEU:HD13	3:L:392:LEU:HD11	2.00	0.43
3:L:418:LEU:HB3	3:L:422:PHE:CE1	2.53	0.43
1:C:179:VAL:CG2	1:C:294:LEU:HD23	2.49	0.43
3:D:769:THR:CG2	3:D:778:VAL:HG13	2.49	0.43
2:G:880:LEU:CD2	2:G:920:ILE:HG23	2.49	0.43
2:H:956:ASN:OD1	2:H:966:THR:HA	2.19	0.43
3:J:356:TYR:HB3	3:J:358:PHE:HE1	1.83	0.43
3:K:371:GLU:HG2	3:K:372:LEU:N	2.33	0.43
3:L:457:TYR:HE1	3:L:461:ASN:ND2	2.17	0.43
3:D:396:PRO:C	3:D:397:ALA:O	2.56	0.43
3:J:422:PHE:HA	3:J:424:ASN:H	1.80	0.43
3:L:415:VAL:H	3:L:436:ASN:CB	2.32	0.43
1:C:227:LEU:HD23	1:C:227:LEU:HA	1.82	0.42
3:D:450:SER:OG	3:D:451:VAL:N	2.51	0.42
3:D:766:LEU:HD12	3:D:767:PRO:CD	2.48	0.42
2:I:940:PRO:HA	2:I:942:ASN:N	2.34	0.42
3:J:408:PHE:C	3:J:408:PHE:CD1	2.91	0.42
3:J:415:VAL:H	3:J:436:ASN:HB3	1.84	0.42
1:A:325:ASN:HB2	1:A:326:ASN:HD22	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:173:GLN:O	3:D:176:ILE:CD1	2.67	0.42
1:F:182:TYR:CE2	1:F:237:PRO:HD3	2.54	0.42
1:F:263:GLU:OE1	1:F:263:GLU:HA	2.19	0.42
1:F:380:LEU:HD22	1:F:404:GLN:HG2	2.00	0.42
2:G:956:ASN:OD1	2:G:966:THR:HA	2.20	0.42
2:I:921:VAL:O	2:I:924:PHE:HB3	2.19	0.42
2:I:956:ASN:OD1	2:I:966:THR:HA	2.19	0.42
3:D:150:SER:HA	3:D:152:LEU:CD1	2.50	0.42
3:D:371:GLU:HG2	3:D:372:LEU:N	2.34	0.42
3:D:422:PHE:CA	3:D:424:ASN:N	2.72	0.42
1:F:168:LEU:HD22	1:F:280:ILE:HG23	2.00	0.42
2:G:929:LEU:HB3	2:G:972:LEU:HD11	2.00	0.42
2:I:931:ARG:O	2:I:934:GLU:HG3	2.19	0.42
3:K:354:PHE:HE2	3:K:373:PRO:HG2	1.81	0.42
3:K:413:ASN:HB2	3:K:436:ASN:ND2	2.34	0.42
1:A:158:LEU:HD11	1:A:385:PHE:CE2	2.54	0.42
1:A:336:GLN:HB3	2:B:937:ILE:HD11	2.00	0.42
3:D:365:ASN:OD1	3:D:365:ASN:N	2.49	0.42
3:D:812:ASP:C	3:D:812:ASP:OD1	2.58	0.42
1:E:387:ILE:O	1:E:390:THR:HG23	2.18	0.42
2:G:764:LEU:HD12	2:G:864:PHE:CD1	2.55	0.42
3:J:410:PHE:CG	3:J:410:PHE:O	2.69	0.42
3:K:356:TYR:HD2	3:K:358:PHE:HE1	1.66	0.42
3:K:365:ASN:OD1	3:K:365:ASN:N	2.49	0.42
3:K:809:PHE:HB3	3:K:810:PRO:HA	2.01	0.42
2:B:956:ASN:OD1	2:B:966:THR:HA	2.19	0.42
1:C:311:LEU:HD21	1:C:338:MET:HE1	2.01	0.42
3:J:383:ARG:HG2	3:J:406:LYS:HG3	2.01	0.42
2:B:813:THR:HG22	2:B:814:PRO:CD	2.50	0.42
1:C:265:LEU:O	1:C:268:SER:HB3	2.20	0.42
1:C:325:ASN:HB2	1:C:326:ASN:HD22	1.84	0.42
3:D:445:ILE:HG13	3:D:457:TYR:HD2	1.84	0.42
1:E:202:PHE:HB2	1:E:203:ARG:H	1.44	0.42
1:F:213:MET:O	1:F:217:VAL:HG23	2.19	0.42
1:F:332:TRP:CZ2	1:F:336:GLN:HG3	2.55	0.42
2:I:929:LEU:HB3	2:I:972:LEU:HD11	2.00	0.42
3:K:379:LEU:HB3	3:K:382:LEU:HD13	2.01	0.42
3:K:458:LEU:O	3:K:459:ARG:C	2.57	0.42
3:K:812:ASP:C	3:K:812:ASP:OD1	2.58	0.42
3:L:445:ILE:CD1	3:L:457:TYR:CD2	3.02	0.42
1:C:354:PHE:O	1:C:355:LYS:CB	2.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:170:SER:O	3:D:176:ILE:HD12	2.20	0.42
3:D:374:ALA:C	3:D:376:ILE:N	2.73	0.42
3:D:536:ARG:O	3:D:540:LEU:HG	2.20	0.42
1:E:202:PHE:CZ	1:E:208:TYR:HD1	2.38	0.42
1:E:219:PHE:HZ	3:L:356:TYR:CE2	2.37	0.42
1:E:346:LEU:HD23	1:E:346:LEU:C	2.40	0.42
1:F:202:PHE:HB2	1:F:203:ARG:H	1.45	0.42
3:J:464:GLU:HB3	3:J:465:ILE:H	1.57	0.42
3:K:551:LEU:HD21	3:K:601:ILE:CG2	2.50	0.42
2:G:910:ILE:HG22	2:G:914:LYS:HE2	2.01	0.42
2:G:942:ASN:OD1	2:G:944:TRP:HB3	2.20	0.42
3:K:163:LEU:HD23	3:K:163:LEU:HA	1.79	0.42
3:K:459:ARG:HD3	3:K:524:ARG:O	2.20	0.42
3:L:423:GLY:H	3:L:458:LEU:HB2	1.85	0.42
1:A:193:GLY:C	1:A:195:LEU:HD23	2.40	0.42
3:D:353:ILE:O	3:D:356:TYR:HB2	2.19	0.42
1:E:184:HIS:O	1:E:229:LEU:HA	2.20	0.42
1:E:256:ILE:HG23	3:L:346:ILE:HD11	2.01	0.42
1:F:154:PRO:HG2	1:F:157:TYR:CG	2.54	0.42
2:H:813:THR:HB	2:H:815:ASN:OD1	2.20	0.42
2:H:867:LEU:HD13	2:H:908:MET:HE1	2.02	0.42
3:L:418:LEU:CD1	3:L:454:LEU:HD21	2.49	0.42
1:C:354:PHE:CZ	1:C:415:ASN:ND2	2.88	0.42
3:D:157:TRP:CZ3	3:D:443:LEU:HD22	2.48	0.42
2:H:837:ASP:O	2:H:840:SER:HB3	2.20	0.42
3:J:369:LEU:N	3:J:390:ASN:OD1	2.52	0.42
3:L:349:ILE:HD13	3:L:349:ILE:HA	1.87	0.42
1:C:350:ILE:CD1	1:C:422:TYR:CZ	3.03	0.41
1:C:354:PHE:HE2	1:C:415:ASN:HB3	1.85	0.41
3:D:514:CYS:SG	3:D:517:TYR:HD1	2.43	0.41
2:G:940:PRO:HA	2:G:942:ASN:N	2.35	0.41
2:H:792:VAL:HG11	2:H:808:LEU:HB2	2.02	0.41
3:J:141:LEU:HD11	3:J:437:PRO:HD3	2.01	0.41
3:J:375:GLU:CD	3:J:375:GLU:H	2.22	0.41
3:K:170:SER:O	3:K:176:ILE:HD12	2.20	0.41
3:K:405:LEU:HD13	3:K:408:PHE:HB2	2.01	0.41
3:L:176:ILE:H	3:L:176:ILE:HG13	1.39	0.41
3:L:364:LEU:HD23	3:L:364:LEU:HA	1.83	0.41
3:L:420:TRP:CD1	3:L:463:PRO:HD2	2.55	0.41
1:A:422:TYR:CD1	1:A:422:TYR:N	2.88	0.41
2:B:813:THR:HB	2:B:815:ASN:OD1	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:166:VAL:HG21	3:D:248:MET:HG3	2.02	0.41
1:E:165:LYS:NZ	1:E:165:LYS:HB3	2.36	0.41
1:E:199:ILE:HG22	1:E:200:GLY:N	2.34	0.41
1:F:380:LEU:HD23	1:F:380:LEU:HA	1.71	0.41
3:J:464:GLU:O	3:J:465:ILE:CB	2.67	0.41
3:K:177:TYR:OH	3:K:386:ASP:OD2	2.39	0.41
3:K:513:LEU:HB3	3:K:536:ARG:NH2	2.35	0.41
3:L:245:GLN:NE2	3:L:409:TYR:CE2	2.88	0.41
3:L:343:ASN:OD1	3:L:366:GLY:HA3	2.19	0.41
1:A:219:PHE:CE1	3:D:356:TYR:CE1	3.08	0.41
3:D:244:LYS:CB	3:D:247:LEU:HB2	2.50	0.41
1:E:354:PHE:HE2	1:E:415:ASN:HB3	1.86	0.41
1:F:193:GLY:O	1:F:195:LEU:HG	2.20	0.41
2:G:977:ASN:O	2:G:978:LEU:HD23	2.20	0.41
3:J:150:SER:CA	3:J:152:LEU:HD12	2.34	0.41
3:L:372:LEU:HA	3:L:373:PRO:HD2	1.82	0.41
3:L:408:PHE:CD1	3:L:408:PHE:C	2.92	0.41
1:A:256:ILE:HG13	3:D:350:SER:H	1.85	0.41
1:A:354:PHE:CE2	1:A:415:ASN:ND2	2.89	0.41
2:B:827:GLN:HA	2:B:827:GLN:OE1	2.21	0.41
3:D:346:ILE:HD12	3:D:367:ASN:ND2	2.35	0.41
3:D:379:LEU:HD23	3:D:379:LEU:HA	1.82	0.41
1:E:325:ASN:HB2	1:E:326:ASN:HD22	1.85	0.41
2:G:803:ASN:O	2:G:806:ASP:N	2.53	0.41
2:G:812:LEU:HD23	2:G:846:MET:HE2	2.02	0.41
2:H:909:LEU:HD21	2:H:925:VAL:HG21	2.02	0.41
2:I:909:LEU:HD12	2:I:951:LEU:HD23	2.03	0.41
3:J:420:TRP:O	3:J:422:PHE:O	2.38	0.41
3:J:422:PHE:CA	3:J:424:ASN:H	2.33	0.41
3:J:444:LYS:O	3:J:447:THR:O	2.38	0.41
3:K:353:ILE:O	3:K:356:TYR:HB2	2.20	0.41
3:K:810:PRO:HB3	3:K:816:SER:N	2.35	0.41
3:L:180:GLN:OE1	3:L:244:LYS:N	2.54	0.41
3:L:379:LEU:HB3	3:L:382:LEU:HD13	2.03	0.41
3:L:392:LEU:O	3:L:413:ASN:HB3	2.21	0.41
1:A:256:ILE:CG1	3:D:350:SER:H	2.34	0.41
1:C:289:LEU:HD23	1:C:318:LEU:HD21	2.01	0.41
1:C:387:ILE:O	1:C:390:THR:HG23	2.20	0.41
3:D:400:GLY:O	3:D:424:ASN:ND2	2.52	0.41
1:E:343:ASP:OD1	1:E:345:ASN:HB3	2.21	0.41
1:E:380:LEU:HA	1:E:380:LEU:HD23	1.71	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:956:ASN:ND2	2:G:966:THR:HG23	2.33	0.41
3:J:349:ILE:HD13	3:J:349:ILE:HA	1.90	0.41
3:K:768:PHE:HA	3:K:778:VAL:HG22	2.03	0.41
3:L:419:PRO:HG2	3:L:422:PHE:CE1	2.55	0.41
1:A:199:ILE:HG22	1:A:200:GLY:N	2.35	0.41
1:A:426:ILE:HG22	1:A:427:TYR:N	2.23	0.41
1:C:258:SER:O	1:C:259:THR:C	2.56	0.41
1:C:332:TRP:CZ2	1:C:336:GLN:HG3	2.56	0.41
3:D:522:MET:C	3:D:523:TYR:CD1	2.94	0.41
3:D:768:PHE:CD1	3:D:768:PHE:N	2.89	0.41
1:F:258:SER:C	1:F:260:GLU:N	2.73	0.41
1:F:314:LEU:HA	1:F:314:LEU:HD12	1.78	0.41
2:H:791:PHE:CE1	2:H:795:ASN:ND2	2.89	0.41
2:H:820:PHE:C	2:H:820:PHE:CD1	2.92	0.41
2:H:929:LEU:HB3	2:H:972:LEU:HD11	2.02	0.41
2:H:979:THR:C	2:H:981:LYS:N	2.74	0.41
2:I:910:ILE:HG22	2:I:914:LYS:HE2	2.02	0.41
3:J:407:TYR:N	3:J:407:TYR:HD1	2.18	0.41
3:K:514:CYS:SG	3:K:517:TYR:HD1	2.43	0.41
3:L:419:PRO:CD	3:L:422:PHE:HE1	2.33	0.41
1:C:287:GLN:HG2	2:H:944:TRP:HA	2.02	0.41
3:D:163:LEU:HD11	3:D:249:GLU:CA	2.41	0.41
2:G:936:LYS:HA	2:G:939:LYS:HE2	2.03	0.41
2:I:909:LEU:HD21	2:I:925:VAL:HG21	2.02	0.41
3:K:369:LEU:HD12	3:K:369:LEU:N	2.36	0.41
3:K:440:LYS:HA	3:K:443:LEU:HB2	2.03	0.41
1:A:184:HIS:O	1:A:229:LEU:HA	2.21	0.41
1:A:301:THR:HG23	1:A:340:ASN:OD1	2.21	0.41
1:C:323:MET:HA	1:C:324:PRO:HD3	1.85	0.41
3:D:254:LEU:HD23	3:D:254:LEU:HA	1.74	0.41
1:E:182:TYR:CE2	1:E:237:PRO:HD3	2.56	0.41
1:E:314:LEU:HD12	1:E:314:LEU:HA	1.78	0.41
1:F:346:LEU:HD23	1:F:350:ILE:HG13	2.03	0.41
3:J:388:SER:CB	3:J:389:HIS:CD2	3.04	0.41
3:J:462:ARG:HA	3:J:463:PRO:HD3	1.70	0.41
3:K:425:LEU:O	3:K:425:LEU:HD12	2.21	0.41
3:K:441:GLN:O	3:K:444:LYS:HB2	2.21	0.41
3:L:163:LEU:HD23	3:L:163:LEU:HA	1.86	0.41
3:L:420:TRP:CZ2	3:L:463:PRO:HD3	2.54	0.41
1:A:182:TYR:CE2	1:A:237:PRO:HD3	2.56	0.41
1:A:311:LEU:HD21	1:A:338:MET:HE1	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:911:GLU:O	2:B:915:GLU:HG2	2.20	0.41
1:C:201:THR:C	1:C:202:PHE:CG	2.93	0.41
1:C:320:ASN:HB3	2:H:941:PRO:O	2.21	0.41
1:C:390:THR:HG1	1:C:393:GLY:H	1.64	0.41
3:D:177:TYR:HE1	3:D:365:ASN:HD21	1.68	0.41
3:D:336:TRP:O	3:D:336:TRP:CG	2.72	0.41
3:D:456:PHE:O	3:D:457:TYR:C	2.56	0.41
3:D:513:LEU:HB3	3:D:536:ARG:NH2	2.36	0.41
1:F:163:VAL:HG12	1:F:280:ILE:HD11	2.02	0.41
2:G:762:ILE:HB	2:G:763:PRO:HD2	2.03	0.41
3:J:346:ILE:HD13	3:J:346:ILE:HG21	1.58	0.41
3:L:397:ALA:C	3:L:399:LEU:N	2.74	0.41
3:L:408:PHE:CD1	3:L:409:TYR:N	2.89	0.41
1:A:179:VAL:CG2	1:A:294:LEU:HD23	2.51	0.41
1:A:214:ARG:HG2	1:A:215:ALA:N	2.34	0.41
1:F:258:SER:O	1:F:260:GLU:N	2.54	0.41
1:F:311:LEU:HD21	1:F:338:MET:HE1	2.03	0.41
3:J:374:ALA:C	3:J:376:ILE:N	2.74	0.41
3:L:423:GLY:CA	3:L:455:ILE:HD12	2.51	0.41
1:A:202:PHE:O	1:A:203:ARG:HG3	2.21	0.40
1:A:258:SER:O	1:A:260:GLU:N	2.54	0.40
1:C:202:PHE:C	1:C:203:ARG:HG3	2.41	0.40
3:D:176:ILE:H	3:D:176:ILE:HG12	1.49	0.40
1:E:225:LEU:C	1:E:225:LEU:HD23	2.42	0.40
1:E:350:ILE:CD1	1:E:422:TYR:CZ	3.04	0.40
3:J:356:TYR:HB3	3:J:358:PHE:CE1	2.56	0.40
3:J:418:LEU:HB3	3:J:422:PHE:CE1	2.55	0.40
3:K:563:GLU:HG2	3:K:563:GLU:H	1.77	0.40
3:K:768:PHE:HA	3:K:777:ASP:O	2.21	0.40
1:A:168:LEU:HD22	1:A:280:ILE:HG23	2.03	0.40
1:A:225:LEU:HD23	1:A:225:LEU:C	2.41	0.40
3:D:135:ASN:HA	3:D:138:ASN:HB2	2.04	0.40
3:D:177:TYR:OH	3:D:386:ASP:OD2	2.40	0.40
3:D:458:LEU:O	3:D:459:ARG:C	2.59	0.40
1:E:402:PHE:CD1	1:E:402:PHE:C	2.94	0.40
2:G:791:PHE:CE1	2:G:795:ASN:ND2	2.90	0.40
3:J:411:PHE:O	3:J:412:ASP:HB3	2.21	0.40
3:K:379:LEU:HD23	3:K:379:LEU:HA	1.78	0.40
3:L:403:PHE:CD1	3:L:403:PHE:C	2.95	0.40
1:A:350:ILE:CD1	1:A:422:TYR:CZ	3.04	0.40
1:C:257:MET:O	3:K:347:PHE:CD1	2.74	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:465:ILE:HD13	3:D:465:ILE:HA	1.85	0.40
3:D:521:LYS:HA	3:D:524:ARG:NH1	2.37	0.40
3:D:522:MET:C	3:D:523:TYR:HD1	2.24	0.40
1:E:305:TYR:O	1:E:306:HIS:HB3	2.20	0.40
2:H:942:ASN:OD1	2:H:944:TRP:HB3	2.21	0.40
3:J:177:TYR:CE2	3:J:363:TYR:CE1	3.10	0.40
3:J:410:PHE:O	3:J:410:PHE:CD2	2.75	0.40
3:L:408:PHE:HD1	3:L:409:TYR:N	2.20	0.40
3:L:414:MET:HA	3:L:437:PRO:HD2	2.03	0.40
3:L:420:TRP:O	3:L:422:PHE:O	2.39	0.40
1:E:346:LEU:HD23	1:E:350:ILE:HG13	2.04	0.40
1:E:354:PHE:CE2	1:E:415:ASN:ND2	2.90	0.40
1:E:405:LEU:HD12	1:E:405:LEU:O	2.21	0.40
1:F:346:LEU:O	1:F:350:ILE:HG13	2.22	0.40
3:K:173:GLN:O	3:K:176:ILE:CD1	2.70	0.40
3:L:341:LEU:O	3:L:344:LEU:HD11	2.21	0.40
1:A:305:TYR:CD1	1:A:344:LEU:HD23	2.57	0.40
1:C:258:SER:C	1:C:260:GLU:N	2.70	0.40
3:D:809:PHE:HB3	3:D:810:PRO:HA	2.03	0.40
1:E:202:PHE:CE1	3:L:336:TRP:CB	3.04	0.40
1:F:185:VAL:HG23	1:F:229:LEU:CD1	2.51	0.40
2:H:861:ARG:O	2:H:864:PHE:HB3	2.21	0.40
3:J:457:TYR:HE1	3:J:461:ASN:ND2	2.19	0.40
3:K:420:TRP:O	3:K:422:PHE:N	2.54	0.40
3:K:768:PHE:CD1	3:K:768:PHE:N	2.90	0.40
3:L:417:THR:HG22	3:L:418:LEU:N	2.37	0.40
3:L:419:PRO:HB2	3:L:421:GLU:HG2	2.03	0.40
3:L:422:PHE:HD2	3:L:425:LEU:HD21	1.86	0.40

All (3) 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)
1:F:166:SER:OG	3:L:146:LEU:O[1_554]	2.08	0.12
2:G:835:TYR:OH	2:I:800:ASN:CA[1_465]	2.10	0.10
1:E:166:SER:OG	3:J:146:LEU:O[1_455]	2.14	0.06

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	263/288 (91%)	250 (95%)	12 (5%)	1 (0%)	34	69
1	C	263/288 (91%)	250 (95%)	12 (5%)	1 (0%)	34	69
1	E	263/288 (91%)	249 (95%)	13 (5%)	1 (0%)	34	69
1	F	263/288 (91%)	250 (95%)	13 (5%)	0	100	100
2	B	231/249 (93%)	222 (96%)	9 (4%)	0	100	100
2	G	231/249 (93%)	222 (96%)	9 (4%)	0	100	100
2	H	231/249 (93%)	221 (96%)	10 (4%)	0	100	100
2	I	231/249 (93%)	222 (96%)	9 (4%)	0	100	100
3	D	300/727 (41%)	253 (84%)	46 (15%)	1 (0%)	41	74
3	J	204/727 (28%)	168 (82%)	34 (17%)	2 (1%)	15	51
3	K	300/727 (41%)	253 (84%)	46 (15%)	1 (0%)	41	74
3	L	204/727 (28%)	171 (84%)	31 (15%)	2 (1%)	15	51
All	All	2984/5056 (59%)	2731 (92%)	244 (8%)	9 (0%)	41	74

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	D	380	SER
3	K	380	SER
3	J	464	GLU
3	J	465	ILE
3	L	465	ILE
1	A	260	GLU
1	C	260	GLU
3	L	464	GLU
1	E	426	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	241/264 (91%)	216 (90%)	25 (10%)	7	30
1	C	242/264 (92%)	218 (90%)	24 (10%)	8	32
1	E	242/264 (92%)	220 (91%)	22 (9%)	9	35
1	F	241/264 (91%)	218 (90%)	23 (10%)	8	33
2	B	211/231 (91%)	199 (94%)	12 (6%)	20	53
2	G	211/231 (91%)	198 (94%)	13 (6%)	18	51
2	H	211/231 (91%)	199 (94%)	12 (6%)	20	53
2	I	211/231 (91%)	198 (94%)	13 (6%)	18	51
3	D	258/648 (40%)	206 (80%)	52 (20%)	1	5
3	J	165/648 (26%)	129 (78%)	36 (22%)	1	4
3	K	261/648 (40%)	208 (80%)	53 (20%)	1	5
3	L	165/648 (26%)	130 (79%)	35 (21%)	1	4
All	All	2659/4572 (58%)	2339 (88%)	320 (12%)	5	23

All (320) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	151	PHE
1	A	152	LEU
1	A	154	PRO
1	A	166	SER
1	A	172	PHE
1	A	180	SER
1	A	184	HIS
1	A	191	PHE
1	A	192	VAL
1	A	202	PHE
1	A	209	HIS
1	A	229	LEU
1	A	255	GLU
1	A	257	MET

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Mol	Chain	Res	Type
1	A	259	THR
1	A	280	ILE
1	A	298	ASP
1	A	323	MET
1	A	327	LYS
1	A	338	MET
1	A	354	PHE
1	A	356	ASN
1	A	374	THR
1	A	386	SER
1	A	426	ILE
2	B	765	LYS
2	B	774	CYS
2	B	813	THR
2	B	820	PHE
2	B	822	THR
2	B	857	ASN
2	B	878	LYS
2	B	901	LYS
2	B	961	TRP
2	B	967	PHE
2	B	968	GLU
2	B	978	LEU
1	C	151	PHE
1	C	152	LEU
1	C	166	SER
1	C	172	PHE
1	C	180	SER
1	C	184	HIS
1	C	191	PHE
1	C	192	VAL
1	C	202	PHE
1	C	209	HIS
1	C	229	LEU
1	C	255	GLU
1	C	257	MET
1	C	259	THR
1	C	280	ILE
1	C	298	ASP
1	C	323	MET
1	C	327	LYS
1	C	338	MET

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Mol	Chain	Res	Type
1	C	355	LYS
1	C	356	ASN
1	C	374	THR
1	C	386	SER
1	C	426	ILE
3	D	141	LEU
3	D	142	HIS
3	D	145	HIS
3	D	176	ILE
3	D	186	TYR
3	D	254	LEU
3	D	255	THR
3	D	256	ASP
3	D	341	LEU
3	D	344	LEU
3	D	347	PHE
3	D	348	ASN
3	D	358	PHE
3	D	359	LEU
3	D	370	THR
3	D	372	LEU
3	D	376	ILE
3	D	377	LYS
3	D	382	LEU
3	D	384	VAL
3	D	398	GLU
3	D	399	LEU
3	D	401	SER
3	D	404	GLN
3	D	416	THR
3	D	422	PHE
3	D	425	LEU
3	D	426	CYS
3	D	436	ASN
3	D	441	GLN
3	D	448	GLU
3	D	455	ILE
3	D	457	TYR
3	D	461	ASN
3	D	467	LEU
3	D	512	THR
3	D	514	CYS

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Mol	Chain	Res	Type
3	D	519	THR
3	D	526	THR
3	D	548	ASP
3	D	554	LEU
3	D	557	VAL
3	D	564	GLU
3	D	565	TYR
3	D	599	CYS
3	D	600	CYS
3	D	777	ASP
3	D	779	ILE
3	D	814	PHE
3	D	817	ASP
3	D	818	HIS
3	D	819	ILE
1	E	151	PHE
1	E	152	LEU
1	E	166	SER
1	E	172	PHE
1	E	180	SER
1	E	184	HIS
1	E	191	PHE
1	E	192	VAL
1	E	202	PHE
1	E	209	HIS
1	E	229	LEU
1	E	255	GLU
1	E	259	THR
1	E	298	ASP
1	E	323	MET
1	E	327	LYS
1	E	338	MET
1	E	354	PHE
1	E	356	ASN
1	E	374	THR
1	E	386	SER
1	E	426	ILE
1	F	151	PHE
1	F	152	LEU
1	F	166	SER
1	F	172	PHE
1	F	180	SER

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Mol	Chain	Res	Type
1	F	184	HIS
1	F	191	PHE
1	F	192	VAL
1	F	202	PHE
1	F	209	HIS
1	F	229	LEU
1	F	255	GLU
1	F	257	MET
1	F	259	THR
1	F	298	ASP
1	F	323	MET
1	F	327	LYS
1	F	338	MET
1	F	354	PHE
1	F	356	ASN
1	F	374	THR
1	F	386	SER
1	F	426	ILE
2	G	765	LYS
2	G	774	CYS
2	G	813	THR
2	G	820	PHE
2	G	822	THR
2	G	857	ASN
2	G	878	LYS
2	G	901	LYS
2	G	961	TRP
2	G	967	PHE
2	G	968	GLU
2	G	978	LEU
2	G	983	LEU
2	H	765	LYS
2	H	774	CYS
2	H	813	THR
2	H	820	PHE
2	H	822	THR
2	H	857	ASN
2	H	878	LYS
2	H	901	LYS
2	H	961	TRP
2	H	967	PHE
2	H	968	GLU

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Mol	Chain	Res	Type
2	H	978	LEU
2	I	765	LYS
2	I	774	CYS
2	I	813	THR
2	I	820	PHE
2	I	822	THR
2	I	857	ASN
2	I	878	LYS
2	I	901	LYS
2	I	961	TRP
2	I	967	PHE
2	I	968	GLU
2	I	978	LEU
2	I	983	LEU
3	J	146	LEU
3	J	147	ASP
3	J	151	LEU
3	J	152	LEU
3	J	175	ASN
3	J	176	ILE
3	J	183	MET
3	J	256	ASP
3	J	341	LEU
3	J	344	LEU
3	J	345	GLN
3	J	346	ILE
3	J	348	ASN
3	J	349	ILE
3	J	358	PHE
3	J	375	GLU
3	J	378	ASN
3	J	381	ASN
3	J	383	ARG
3	J	384	VAL
3	J	393	THR
3	J	394	SER
3	J	398	GLU
3	J	401	SER
3	J	404	GLN
3	J	407	TYR
3	J	408	PHE
3	J	422	PHE

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Mol	Chain	Res	Type
3	J	425	LEU
3	J	426	CYS
3	J	436	ASN
3	J	443	LEU
3	J	444	LYS
3	J	452	THR
3	J	456	PHE
3	J	461	ASN
3	K	141	LEU
3	K	142	HIS
3	K	145	HIS
3	K	176	ILE
3	K	186	TYR
3	K	254	LEU
3	K	255	THR
3	K	256	ASP
3	K	341	LEU
3	K	344	LEU
3	K	347	PHE
3	K	348	ASN
3	K	358	PHE
3	K	359	LEU
3	K	370	THR
3	K	372	LEU
3	K	376	ILE
3	K	377	LYS
3	K	382	LEU
3	K	384	VAL
3	K	398	GLU
3	K	399	LEU
3	K	401	SER
3	K	404	GLN
3	K	409	TYR
3	K	416	THR
3	K	422	PHE
3	K	425	LEU
3	K	426	CYS
3	K	436	ASN
3	K	441	GLN
3	K	448	GLU
3	K	455	ILE
3	K	457	TYR

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Mol	Chain	Res	Type
3	K	461	ASN
3	K	467	LEU
3	K	512	THR
3	K	514	CYS
3	K	516	HIS
3	K	519	THR
3	K	526	THR
3	K	548	ASP
3	K	554	LEU
3	K	557	VAL
3	K	564	GLU
3	K	565	TYR
3	K	597	ASP
3	K	777	ASP
3	K	779	ILE
3	K	814	PHE
3	K	817	ASP
3	K	818	HIS
3	K	819	ILE
3	L	139	PRO
3	L	147	ASP
3	L	151	LEU
3	L	152	LEU
3	L	175	ASN
3	L	176	ILE
3	L	183	MET
3	L	256	ASP
3	L	341	LEU
3	L	344	LEU
3	L	345	GLN
3	L	346	ILE
3	L	349	ILE
3	L	358	PHE
3	L	375	GLU
3	L	378	ASN
3	L	381	ASN
3	L	383	ARG
3	L	384	VAL
3	L	393	THR
3	L	394	SER
3	L	398	GLU
3	L	401	SER

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Mol	Chain	Res	Type
3	L	404	GLN
3	L	407	TYR
3	L	408	PHE
3	L	422	PHE
3	L	425	LEU
3	L	426	CYS
3	L	436	ASN
3	L	443	LEU
3	L	444	LYS
3	L	452	THR
3	L	456	PHE
3	L	461	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	287	GLN
1	C	287	GLN
3	D	343	ASN
3	D	413	ASN
3	D	424	ASN
3	K	352	ASN
3	K	413	ASN
3	K	424	ASN
3	L	175	ASN

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 monosaccharides 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	267/288 (92%)	-0.19	1 (0%)	92	91	36, 58, 98, 121	0
1	C	267/288 (92%)	-0.18	2 (0%)	87	86	36, 58, 99, 121	0
1	E	267/288 (92%)	-0.25	0	100	100	35, 58, 100, 121	0
1	F	267/288 (92%)	-0.20	1 (0%)	92	91	36, 59, 98, 124	0
2	B	233/249 (93%)	0.00	3 (1%)	77	75	48, 79, 115, 146	0
2	G	233/249 (93%)	-0.10	2 (0%)	84	83	49, 81, 112, 146	0
2	H	233/249 (93%)	0.04	5 (2%)	63	63	48, 80, 115, 145	0
2	I	233/249 (93%)	-0.06	5 (2%)	63	63	50, 81, 114, 145	0
3	D	318/727 (43%)	0.11	14 (4%)	34	34	50, 87, 136, 160	0
3	J	210/727 (28%)	-0.29	4 (1%)	66	66	35, 61, 101, 127	0
3	K	318/727 (43%)	0.19	22 (6%)	16	20	50, 87, 136, 160	0
3	L	210/727 (28%)	-0.23	3 (1%)	75	73	35, 62, 102, 131	0
All	All	3056/5056 (60%)	-0.08	62 (2%)	65	64	35, 72, 115, 160	0

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	K	597	ASP	5.4
3	K	135	ASN	4.1
2	H	801	LEU	3.8
2	B	991	THR	3.8
3	K	149	PRO	3.6
3	K	517	TYR	3.6
1	C	355	LYS	3.5
1	A	371	TYR	3.3
2	H	991	THR	3.3
3	K	259	THR	3.3
3	L	466	PRO	3.2

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Mol	Chain	Res	Type	RSRZ
3	D	259	THR	3.2
2	I	961	TRP	3.2
3	K	598	GLY	3.2
3	D	135	ASN	3.2
3	K	551	LEU	3.2
2	H	805	VAL	3.1
3	K	145	HIS	3.0
3	D	257	SER	3.0
3	K	557	VAL	3.0
3	K	596	VAL	2.9
3	K	603	PHE	2.8
3	L	423	GLY	2.8
3	D	551	LEU	2.7
3	K	516	HIS	2.7
2	I	989	ILE	2.7
1	C	371	TYR	2.7
2	G	872	GLU	2.6
3	K	562	PHE	2.6
3	J	187	LEU	2.5
2	I	956	ASN	2.5
3	K	778	VAL	2.5
3	D	242	CYS	2.5
2	B	782	PRO	2.5
2	H	809	LYS	2.5
3	D	597	ASP	2.5
3	D	801	GLU	2.5
3	D	255	THR	2.4
2	I	872	GLU	2.4
3	D	149	PRO	2.4
3	J	149	PRO	2.4
3	K	242	CYS	2.3
3	K	518	ALA	2.3
3	D	137	SER	2.3
3	D	550	ASP	2.3
2	I	791	PHE	2.3
3	K	257	SER	2.3
3	D	598	GLY	2.2
2	B	784	ASP	2.2
3	D	562	PHE	2.2
3	K	137	SER	2.2
3	K	766	LEU	2.2
2	G	870	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	F	414	PRO	2.2
3	K	143	PRO	2.2
3	K	601	ILE	2.1
3	D	800	PRO	2.1
3	J	252	ASP	2.1
3	K	554	LEU	2.1
3	L	149	PRO	2.1
2	H	808	LEU	2.0
3	J	186	TYR	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 monosaccharides 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.