



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2018 – 11:28 pm GMT

PDB ID : 4XR7
Title : Structure of the *Saccharomyces cerevisiae* PAN2-PAN3 core complex
Authors : Schafer, I.B.; Rode, M.; Bonneau, F.; Schussler, S.; Conti, E.
Deposited on : 2015-01-20
Resolution : 3.80 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 : trunk30967
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk30967

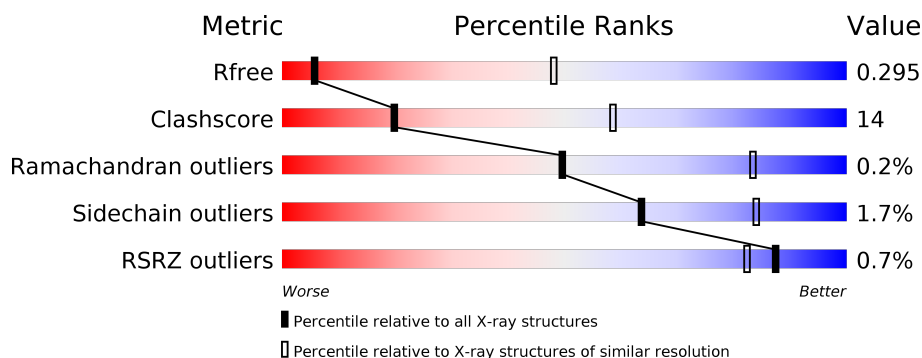
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	111664	1028 (4.02-3.58)
Clashscore	122126	1061 (4.00-3.60)
Ramachandran outliers	120053	1025 (4.00-3.60)
Sidechain outliers	120020	1019 (4.00-3.60)
RSRZ outliers	108989	1021 (4.06-3.54)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	776	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 68%, green 22%, grey 10%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> % 68% 22% • 10% </div> </div>
1	D	776	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 67%, green 20%, grey 12%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> % 67% 20% • 12% </div> </div>
1	G	776	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 67%, green 21%, grey 12%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> % 67% 21% 12% </div> </div>
1	J	776	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 65%, green 22%, grey 12%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> % 65% 22% • 12% </div> </div>
2	B	465	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, green 62%, yellow 29%, grey 8%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 62% 29% • 8% </div> </div>
2	C	465	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 63%, green 31%, grey 5%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> % 63% 31% • 5% </div> </div>

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Mol	Chain	Length	Quality of chain
2	E	465	<div><div></div><div>62%27%11%</div></div>
2	F	465	<div><div></div><div>63%31%5%</div></div>
2	H	465	<div><div></div><div>61%28%10%</div></div>
2	I	465	<div><div></div><div>%59%34%6%</div></div>
2	K	465	<div><div></div><div>2%68%24%7%</div></div>
2	L	465	<div><div></div><div>60%35%5%</div></div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 46467 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 PAB-dependent poly(A)-specific ribonuclease subunit PAN2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	G	683	Total	C	N	O	S	0	0	0
			4981	3160	829	972	20			
1	D	683	Total	C	N	O	S	0	0	0
			4973	3153	834	966	20			
1	J	681	Total	C	N	O	S	0	0	0
			4958	3162	810	967	19			
1	A	701	Total	C	N	O	S	0	0	0
			5217	3323	860	1012	22			

- Molecule 2 is a protein called PAB-dependent poly(A)-specific ribonuclease subunit PAN3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	441	Total	C	N	O	S	0	0	0
			3479	2243	576	646	14			
2	K	431	Total	C	N	O	S	0	0	0
			3272	2087	547	624	14			
2	E	414	Total	C	N	O	S	0	0	0
			3084	1985	509	576	14			
2	F	442	Total	C	N	O	S	0	0	0
			3381	2186	553	628	14			
2	H	420	Total	C	N	O	S	0	0	0
			3153	2020	523	596	14			
2	I	437	Total	C	N	O	S	0	0	0
			3292	2109	541	628	14			
2	C	444	Total	C	N	O	S	0	0	0
			3405	2188	561	642	14			
2	B	429	Total	C	N	O	S	0	0	0
			3272	2093	545	620	14			

There are 88 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	225	MET	-	initiating methionine	UNP P36102

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Chain	Residue	Modelled	Actual	Comment	Reference
L	680	HIS	-	expression tag	UNP P36102
L	681	HIS	-	expression tag	UNP P36102
L	682	HIS	-	expression tag	UNP P36102
L	683	HIS	-	expression tag	UNP P36102
L	684	HIS	-	expression tag	UNP P36102
L	685	HIS	-	expression tag	UNP P36102
L	686	HIS	-	expression tag	UNP P36102
L	687	HIS	-	expression tag	UNP P36102
L	688	HIS	-	expression tag	UNP P36102
L	689	HIS	-	expression tag	UNP P36102
K	219	MET	-	initiating methionine	UNP P36102
K	680	HIS	-	expression tag	UNP P36102
K	681	HIS	-	expression tag	UNP P36102
K	682	HIS	-	expression tag	UNP P36102
K	683	HIS	-	expression tag	UNP P36102
K	684	HIS	-	expression tag	UNP P36102
K	685	HIS	-	expression tag	UNP P36102
K	686	HIS	-	expression tag	UNP P36102
K	687	HIS	-	expression tag	UNP P36102
K	688	HIS	-	expression tag	UNP P36102
K	689	HIS	-	expression tag	UNP P36102
E	225	MET	-	initiating methionine	UNP P36102
E	680	HIS	-	expression tag	UNP P36102
E	681	HIS	-	expression tag	UNP P36102
E	682	HIS	-	expression tag	UNP P36102
E	683	HIS	-	expression tag	UNP P36102
E	684	HIS	-	expression tag	UNP P36102
E	685	HIS	-	expression tag	UNP P36102
E	686	HIS	-	expression tag	UNP P36102
E	687	HIS	-	expression tag	UNP P36102
E	688	HIS	-	expression tag	UNP P36102
E	689	HIS	-	expression tag	UNP P36102
F	225	MET	-	initiating methionine	UNP P36102
F	680	HIS	-	expression tag	UNP P36102
F	681	HIS	-	expression tag	UNP P36102
F	682	HIS	-	expression tag	UNP P36102
F	683	HIS	-	expression tag	UNP P36102
F	684	HIS	-	expression tag	UNP P36102
F	685	HIS	-	expression tag	UNP P36102
F	686	HIS	-	expression tag	UNP P36102
F	687	HIS	-	expression tag	UNP P36102
F	688	HIS	-	expression tag	UNP P36102

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Chain	Residue	Modelled	Actual	Comment	Reference
F	689	HIS	-	expression tag	UNP P36102
H	225	MET	-	initiating methionine	UNP P36102
H	680	HIS	-	expression tag	UNP P36102
H	681	HIS	-	expression tag	UNP P36102
H	682	HIS	-	expression tag	UNP P36102
H	683	HIS	-	expression tag	UNP P36102
H	684	HIS	-	expression tag	UNP P36102
H	685	HIS	-	expression tag	UNP P36102
H	686	HIS	-	expression tag	UNP P36102
H	687	HIS	-	expression tag	UNP P36102
H	688	HIS	-	expression tag	UNP P36102
H	689	HIS	-	expression tag	UNP P36102
I	225	MET	-	initiating methionine	UNP P36102
I	680	HIS	-	expression tag	UNP P36102
I	681	HIS	-	expression tag	UNP P36102
I	682	HIS	-	expression tag	UNP P36102
I	683	HIS	-	expression tag	UNP P36102
I	684	HIS	-	expression tag	UNP P36102
I	685	HIS	-	expression tag	UNP P36102
I	686	HIS	-	expression tag	UNP P36102
I	687	HIS	-	expression tag	UNP P36102
I	688	HIS	-	expression tag	UNP P36102
I	689	HIS	-	expression tag	UNP P36102
C	225	MET	-	initiating methionine	UNP P36102
C	680	HIS	-	expression tag	UNP P36102
C	681	HIS	-	expression tag	UNP P36102
C	682	HIS	-	expression tag	UNP P36102
C	683	HIS	-	expression tag	UNP P36102
C	684	HIS	-	expression tag	UNP P36102
C	685	HIS	-	expression tag	UNP P36102
C	686	HIS	-	expression tag	UNP P36102
C	687	HIS	-	expression tag	UNP P36102
C	688	HIS	-	expression tag	UNP P36102
C	689	HIS	-	expression tag	UNP P36102
B	225	MET	-	initiating methionine	UNP P36102
B	680	HIS	-	expression tag	UNP P36102
B	681	HIS	-	expression tag	UNP P36102
B	682	HIS	-	expression tag	UNP P36102
B	683	HIS	-	expression tag	UNP P36102
B	684	HIS	-	expression tag	UNP P36102
B	685	HIS	-	expression tag	UNP P36102
B	686	HIS	-	expression tag	UNP P36102

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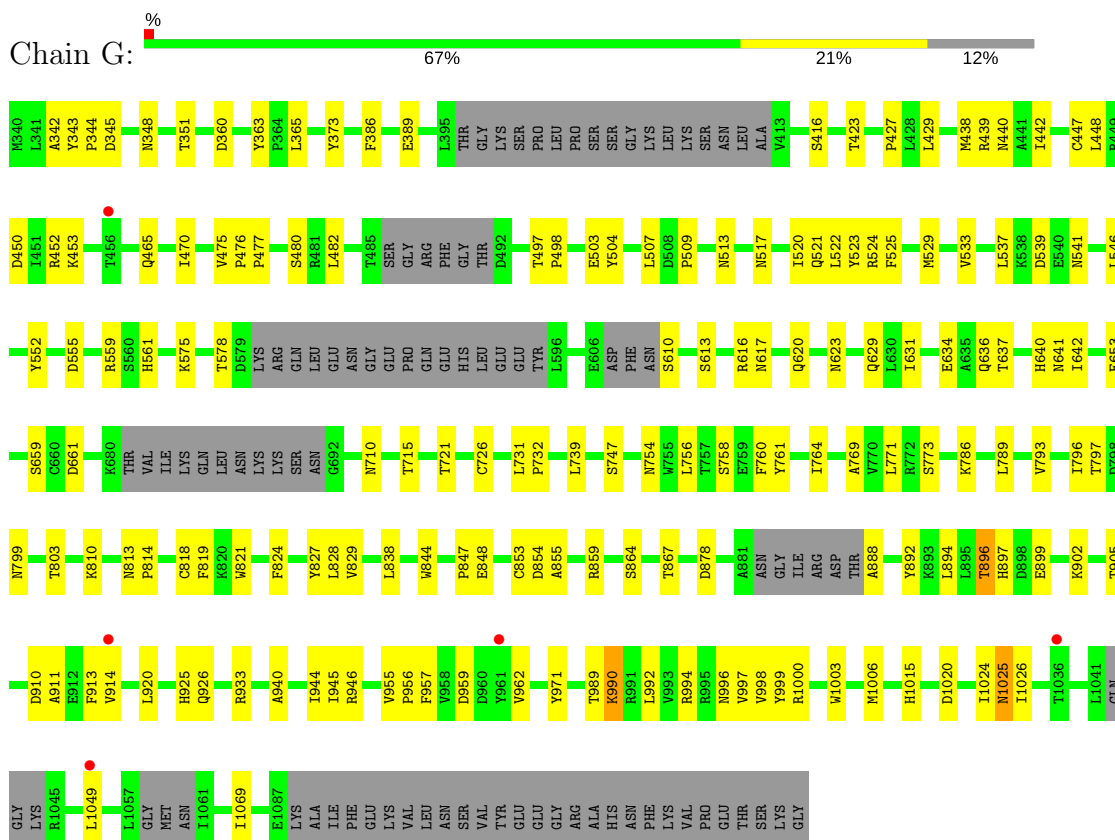
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Chain	Residue	Modelled	Actual	Comment	Reference
B	687	HIS	-	expression tag	UNP P36102
B	688	HIS	-	expression tag	UNP P36102
B	689	HIS	-	expression tag	UNP P36102

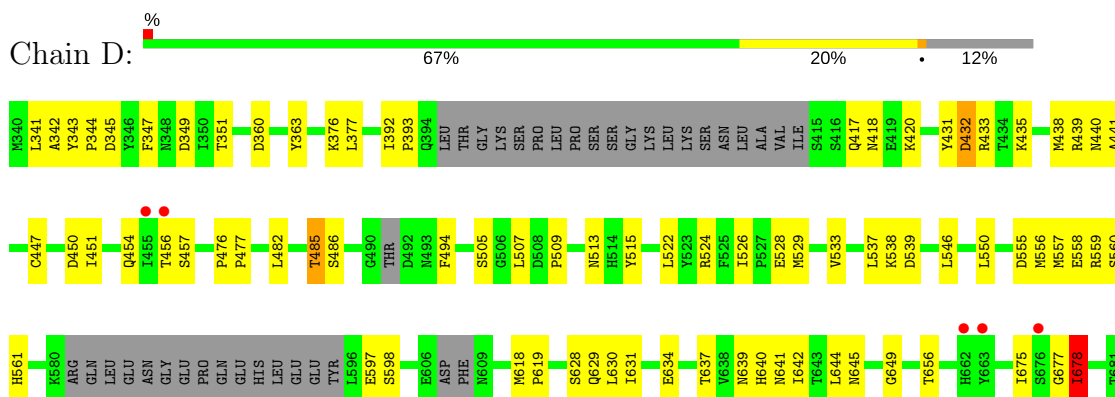
3 Residue-property plots

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.

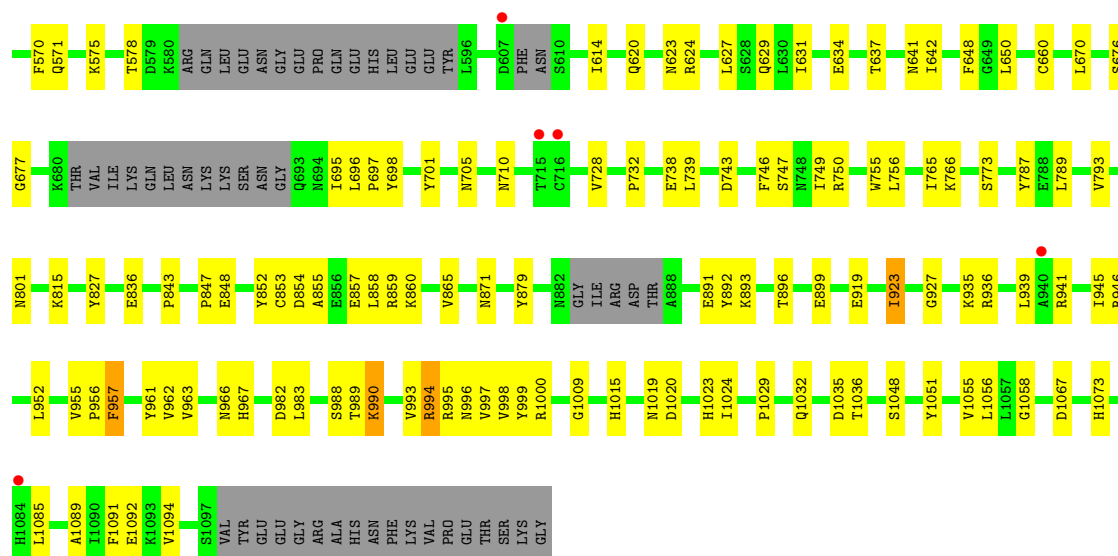
- Molecule 1: PAB-dependent poly(A)-specific ribonuclease subunit PAN2



- Molecule 1: PAB-dependent poly(A)-specific ribonuclease subunit PAN2

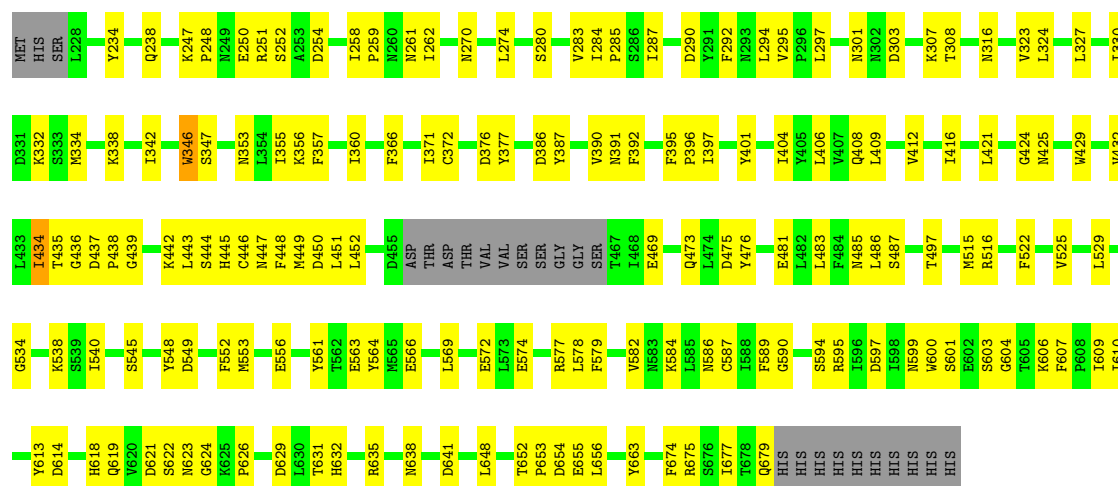






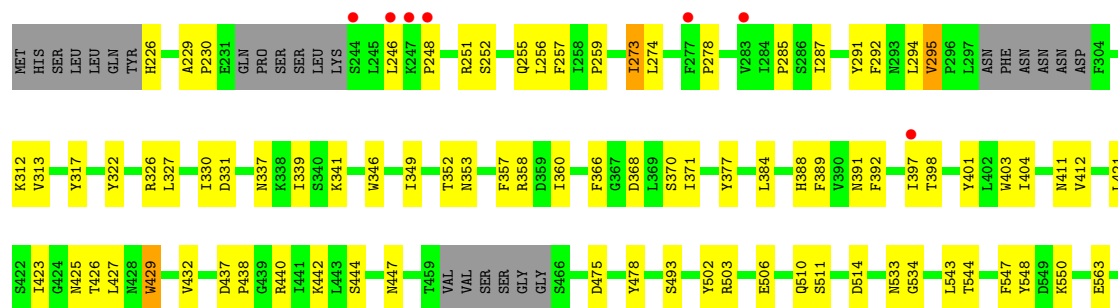
• Molecule 2: PAB-dependent poly(A)-specific ribonuclease subunit PAN3

Chain L: 60% 35% 5%



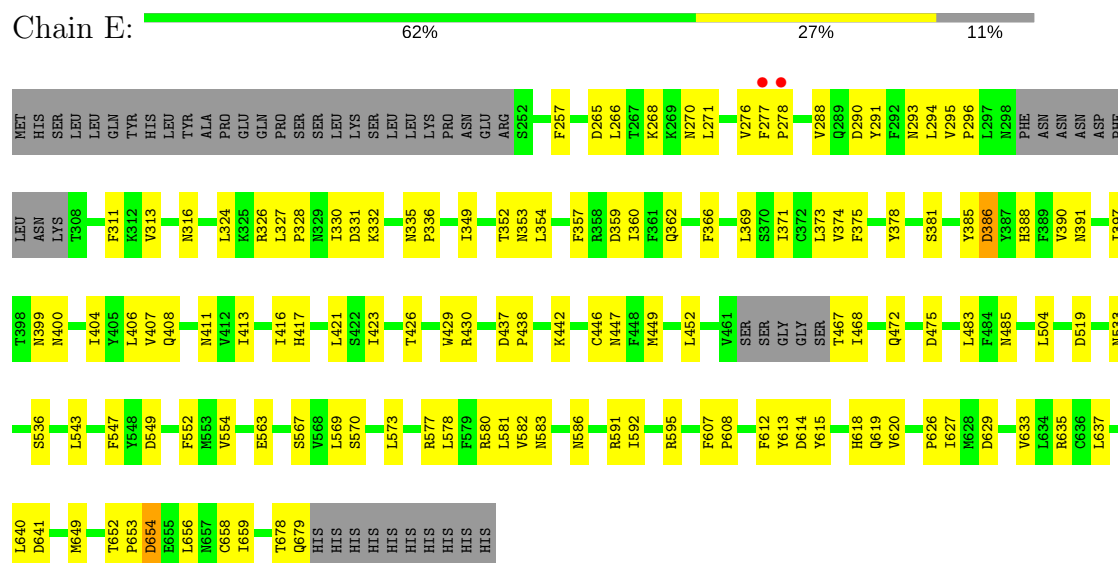
• Molecule 2: PAB-dependent poly(A)-specific ribonuclease subunit PAN3

Chain K: 2% 68% 24% 7%

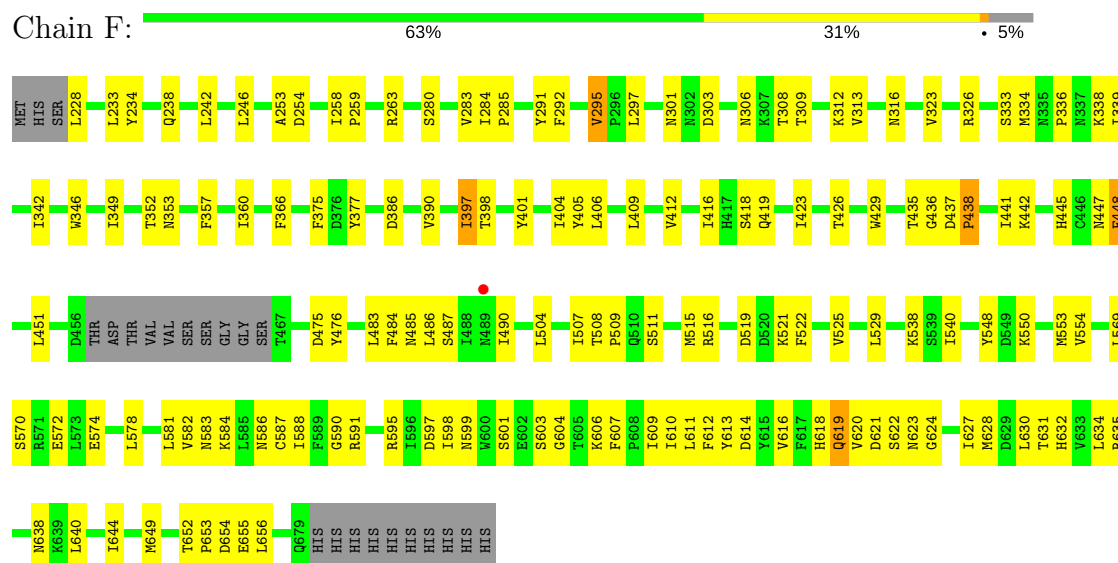




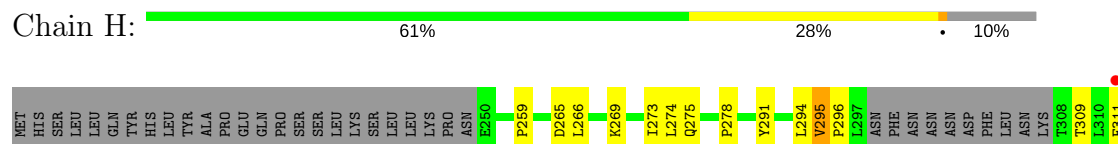
• Molecule 2: PAB-dependent poly(A)-specific ribonuclease subunit PAN3

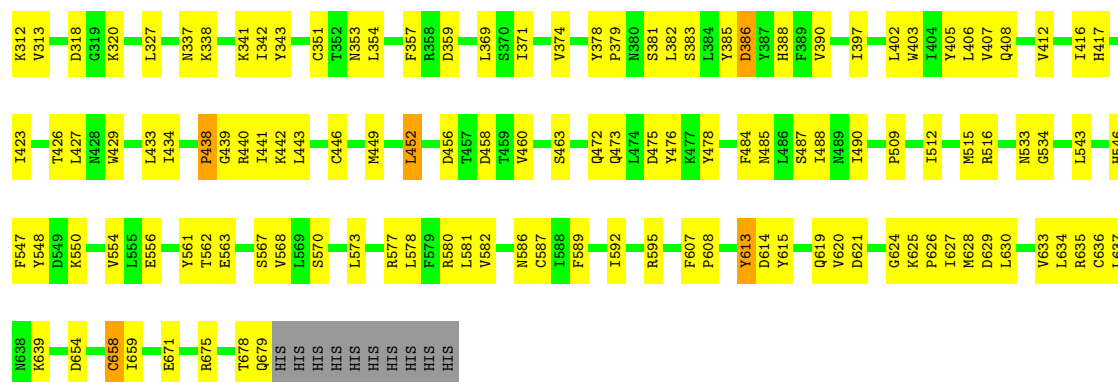


• Molecule 2: PAB-dependent poly(A)-specific ribonuclease subunit PAN3

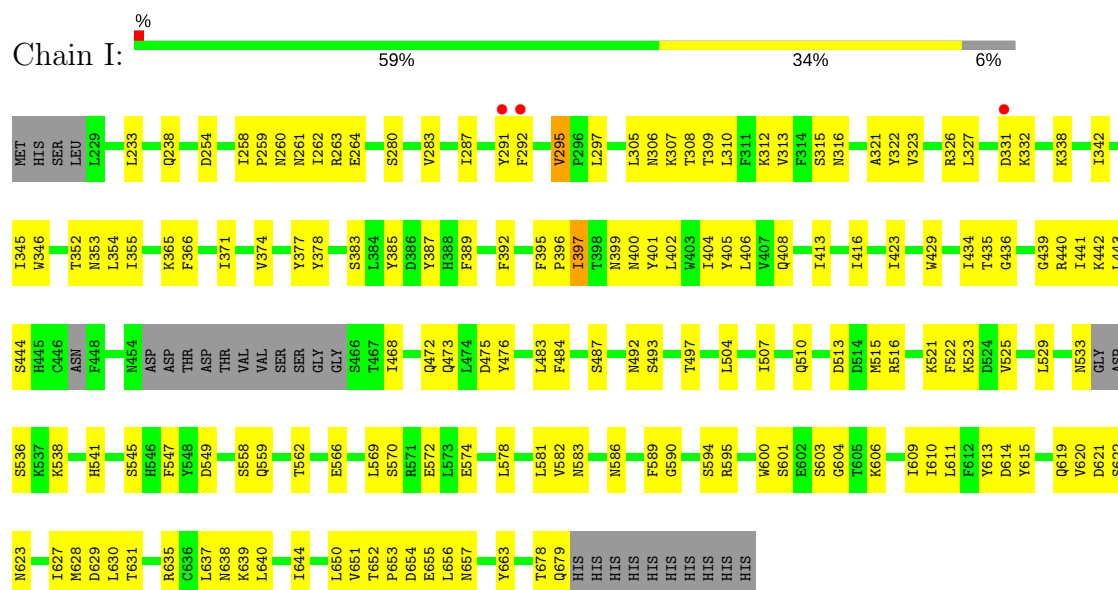


• Molecule 2: PAB-dependent poly(A)-specific ribonuclease subunit PAN3

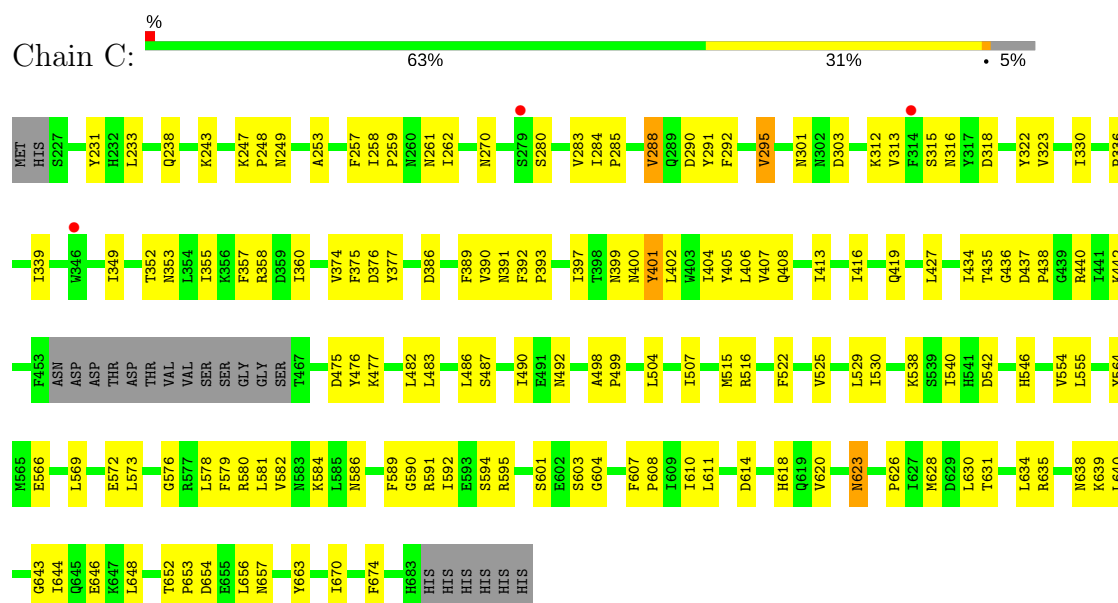




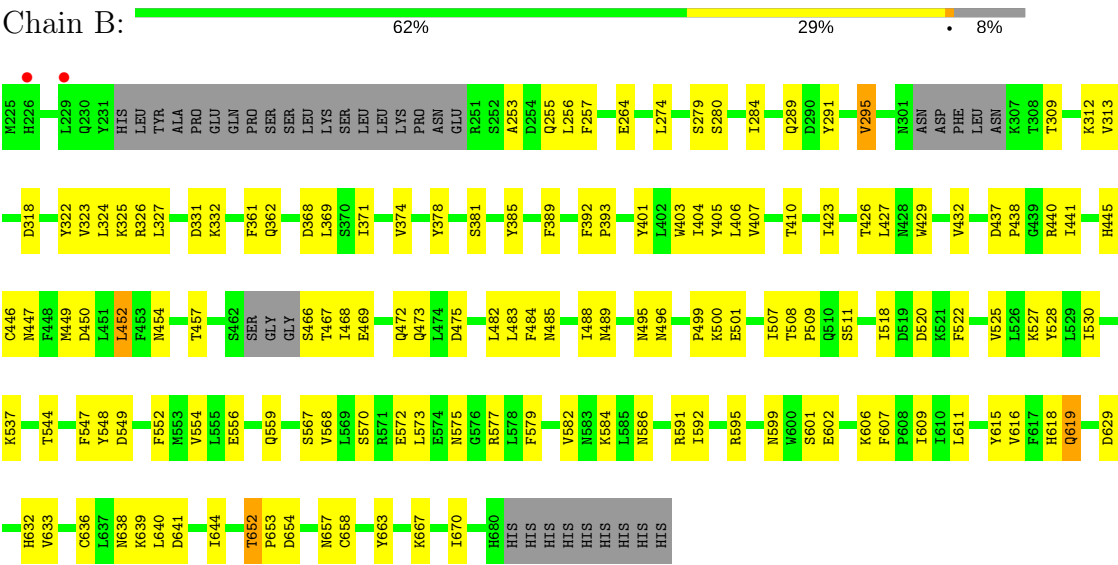
• Molecule 2: PAB-dependent poly(A)-specific ribonuclease subunit PAN3



• Molecule 2: PAB-dependent poly(A)-specific ribonuclease subunit PAN3



● Molecule 2: PAB-dependent poly(A)-specific ribonuclease subunit PAN3



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	131.44Å 205.30Å 234.41Å 90.00° 94.10° 90.00°	Depositor
Resolution (Å)	48.83 – 3.80 48.83 – 3.79	Depositor EDS
% Data completeness (in resolution range)	99.0 (48.83-3.80) 99.3 (48.83-3.79)	Depositor EDS
R_{merge}	0.38	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.50 (at 3.77Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.285 , 0.299 0.281 , 0.295	Depositor DCC
R_{free} test set	6098 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	133.3	Xtriage
Anisotropy	0.288	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 71.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	46467	wwPDB-VP
Average B, all atoms (Å ²)	114.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.26% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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	0.28	0/5327	0.56	0/7277
1	D	0.28	0/5074	0.55	1/6935 (0.0%)
1	G	0.29	0/5080	0.57	1/6945 (0.0%)
1	J	0.28	0/5062	0.56	0/6924
2	B	0.32	0/3341	0.65	3/4547 (0.1%)
2	C	0.28	0/3483	0.58	0/4752
2	E	0.31	0/3150	0.61	1/4298 (0.0%)
2	F	0.29	0/3459	0.59	0/4723
2	H	0.30	0/3221	0.63	3/4392 (0.1%)
2	I	0.29	0/3365	0.58	1/4595 (0.0%)
2	K	0.30	0/3341	0.63	3/4550 (0.1%)
2	L	0.29	0/3558	0.60	1/4837 (0.0%)
All	All	0.29	0/47461	0.59	14/64775 (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	4
1	D	0	2
1	G	0	1
1	J	0	2
2	C	0	1
2	F	0	1
2	H	0	1
2	L	0	1
All	All	0	13

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	452	LEU	CA-CB-CG	7.63	132.86	115.30
2	B	652	THR	C-N-CD	-7.10	104.98	120.60
2	K	652	THR	C-N-CD	-6.95	105.30	120.60
1	G	561	HIS	N-CA-C	-6.43	93.63	111.00
2	L	534	GLY	N-CA-C	-6.28	97.40	113.10
2	K	230	PRO	N-CA-CB	6.00	110.50	103.30
2	E	654	ASP	N-CA-C	-5.47	96.22	111.00
2	H	452	LEU	CA-CB-CG	5.45	127.84	115.30
2	H	654	ASP	N-CA-C	-5.42	96.36	111.00
2	H	439	GLY	N-CA-C	5.42	126.64	113.10
2	B	652	THR	C-N-CA	5.38	144.60	122.00
2	K	652	THR	C-N-CA	5.26	144.08	122.00
2	I	392	PHE	C-N-CD	5.22	139.36	128.40
1	D	432	ASP	N-CA-C	5.03	124.57	111.00

There are no chirality outliers.

All (13) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1058	GLY	Peptide
1	A	422	SER	Peptide
1	A	430	ARG	Peptide
1	A	994	ARG	Peptide
2	C	288	VAL	Peptide
1	D	431	TYR	Peptide
1	D	994	ARG	Peptide
2	F	438	PRO	Peptide
1	G	453	LYS	Peptide
2	H	456	ASP	Peptide
1	J	421	LEU	Peptide
1	J	495	ASP	Peptide
2	L	366	PHE	Peptide

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	5217	0	4654	115	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	4973	0	4313	105	0
1	G	4981	0	4348	115	0
1	J	4958	0	4283	124	0
2	B	3272	0	2970	107	0
2	C	3405	0	3129	119	0
2	E	3084	0	2749	96	0
2	F	3381	0	3120	124	0
2	H	3153	0	2811	97	0
2	I	3292	0	2945	127	0
2	K	3272	0	2943	97	0
2	L	3479	0	3315	127	0
All	All	46467	0	41580	1198	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 14.

All (1198) 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)
2:I:353:ASN:HA	2:I:442:LYS:HG2	1.55	0.89
2:K:256:LEU:HD13	2:K:404:ILE:HD11	1.56	0.87
2:H:586:ASN:OD1	2:I:586:ASN:ND2	2.08	0.85
2:K:577:ARG:NH1	1:J:370:MET:SD	2.49	0.85
2:B:256:LEU:HD13	2:B:404:ILE:HD11	1.60	0.83
1:J:1009:GLY:HA2	1:J:1032:GLN:HE22	1.43	0.83
2:I:611:LEU:HD22	2:I:650:LEU:HB3	1.61	0.82
2:C:644:ILE:HG22	2:C:646:GLU:H	1.45	0.82
2:I:594:SER:OG	2:I:600:TRP:O	1.98	0.82
2:L:594:SER:OG	2:L:600:TRP:O	1.95	0.82
2:F:284:ILE:HG12	2:F:285:PRO:HD2	1.61	0.81
1:G:996:ASN:O	1:G:1000:ARG:N	2.13	0.81
1:G:429:LEU:HD12	2:I:657:ASN:HB3	1.60	0.81
2:B:518:ILE:HG22	2:B:520:ASP:H	1.44	0.80
2:E:586:ASN:OD1	2:F:586:ASN:ND2	2.11	0.79
1:J:1029:PRO:HG2	1:J:1032:GLN:HG3	1.62	0.79
1:A:1085:LEU:HD21	1:A:1091:PHE:HB3	1.64	0.78
1:A:945:ILE:HA	1:A:956:PRO:HA	1.65	0.78
2:L:586:ASN:ND2	2:K:586:ASN:OD1	2.16	0.78
2:E:352:THR:O	2:E:442:LYS:NZ	2.17	0.78
1:G:747:SER:OG	2:I:623:ASN:OD1	2.02	0.78
2:H:613:TYR:OH	2:I:586:ASN:ND2	2.16	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:623:ASN:ND2	1:A:747:SER:OG	2.14	0.77
2:B:636:CYS:SG	1:A:348:ASN:ND2	2.58	0.77
2:F:516:ARG:NH2	1:A:773:SER:O	2.18	0.77
2:B:295:VAL:HG22	2:B:312:LYS:HB3	1.67	0.77
2:L:346:TRP:NE1	2:L:446:CYS:SG	2.59	0.76
1:G:389:GLU:OE1	2:I:631:THR:OG1	2.02	0.76
2:F:342:ILE:HD12	2:F:451:LEU:HD13	1.67	0.76
2:H:291:TYR:HB3	2:H:313:VAL:HG21	1.68	0.76
2:L:234:TYR:HA	1:J:377:LEU:HD12	1.68	0.76
1:J:620:GLN:NE2	1:J:848:GLU:OE1	2.18	0.76
1:G:773:SER:O	2:L:516:ARG:NH2	2.19	0.75
2:F:426:THR:HG23	2:F:447:ASN:HB2	1.68	0.75
1:G:345:ASP:OD2	2:H:615:TYR:OH	2.04	0.75
2:I:516:ARG:NH2	1:J:773:SER:O	2.20	0.75
2:C:566:GLU:OE1	2:B:440:ARG:NH2	2.20	0.75
1:G:1015:HIS:HB3	1:G:1049:LEU:HD22	1.70	0.74
2:C:397:ILE:HD11	2:C:486:LEU:HB3	1.69	0.74
2:F:285:PRO:HG3	2:F:366:PHE:HE1	1.52	0.74
1:G:465:GLN:NE2	1:G:498:PRO:O	2.19	0.74
1:A:919:GLU:HB2	1:A:935:LYS:HG3	1.69	0.74
1:J:962:VAL:HG23	1:J:994:ARG:HB3	1.70	0.74
1:G:959:ASP:OD1	1:G:990:LYS:NZ	2.20	0.73
1:J:996:ASN:O	1:J:1000:ARG:N	2.20	0.73
2:L:386:ASP:HA	2:L:390:VAL:HG22	1.69	0.73
2:E:385:TYR:HB2	2:E:429:TRP:CD1	2.24	0.73
2:H:275:GLN:HG3	2:I:644:ILE:HD13	1.70	0.73
2:C:631:THR:OG1	1:A:389:GLU:OE1	2.06	0.73
2:L:595:ARG:NH2	2:K:614:ASP:OD2	2.21	0.73
2:H:440:ARG:NH2	2:I:566:GLU:OE1	2.20	0.73
1:A:620:GLN:NE2	1:A:848:GLU:OE1	2.22	0.72
2:F:574:GLU:OE2	2:F:638:ASN:ND2	2.22	0.72
2:I:331:ASP:OD1	2:I:332:LYS:N	2.20	0.72
1:D:439:ARG:NH1	1:D:440:ASN:OD1	2.22	0.72
2:E:266:LEU:HD21	2:F:570:SER:HA	1.71	0.72
1:D:597:GLU:OE1	1:D:629:GLN:NE2	2.23	0.71
1:A:941:ARG:NH1	1:A:1067:ASP:OD2	2.23	0.71
2:K:291:TYR:HB3	2:K:313:VAL:HG21	1.72	0.71
2:C:482:LEU:HD22	2:C:483:LEU:HD12	1.71	0.71
2:L:284:ILE:HG12	2:L:285:PRO:HD2	1.70	0.71
2:E:614:ASP:OD2	2:F:595:ARG:NH2	2.22	0.71
1:G:348:ASN:ND2	2:H:636:CYS:SG	2.64	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:763:SER:HB2	1:J:784:ILE:HA	1.72	0.71
1:J:439:ARG:NH1	1:J:440:ASN:OD1	2.24	0.71
2:H:385:TYR:HB2	2:H:429:TRP:CD1	2.26	0.70
1:J:874:ILE:HG21	1:J:1000:ARG:HG2	1.72	0.70
2:E:331:ASP:OD1	2:E:332:LYS:N	2.24	0.70
2:B:385:TYR:HB2	2:B:429:TRP:CD1	2.27	0.70
2:L:301:ASN:HD22	2:L:308:THR:HA	1.55	0.70
2:C:291:TYR:HB3	2:C:313:VAL:HG21	1.72	0.70
2:L:574:GLU:OE2	2:L:638:ASN:ND2	2.25	0.69
2:L:481:GLU:O	2:L:485:ASN:ND2	2.25	0.69
2:B:485:ASN:HD21	2:B:501:GLU:HA	1.57	0.69
2:B:619:GLN:HE21	1:A:343:TYR:HB2	1.57	0.69
1:J:513:ASN:OD1	1:J:571:GLN:NE2	2.26	0.69
2:I:280:SER:HB2	2:I:283:VAL:HG12	1.75	0.69
2:I:287:ILE:HD12	2:I:292:PHE:HB3	1.74	0.69
1:A:1092:GLU:HG3	1:A:1094:VAL:H	1.57	0.68
1:D:914:VAL:HG23	1:D:971:TYR:HA	1.75	0.68
1:G:994:ARG:O	1:G:997:VAL:N	2.23	0.68
2:K:357:PHE:HZ	2:K:360:ILE:HB	1.56	0.68
1:A:857:GLU:OE2	1:A:860:LYS:NZ	2.19	0.68
2:I:434:ILE:HD11	2:I:439:GLY:HA2	1.74	0.68
1:D:963:VAL:HG23	1:D:983:LEU:HA	1.75	0.68
2:E:295:VAL:O	2:E:311:PHE:HB2	1.94	0.68
2:L:529:LEU:O	2:L:538:LYS:NZ	2.27	0.68
2:E:426:THR:HG21	2:E:446:CYS:H	1.59	0.68
2:H:615:TYR:O	2:H:619:GLN:NE2	2.27	0.68
1:J:854:ASP:HB3	1:J:857:GLU:HB2	1.74	0.68
2:E:406:LEU:HD13	2:E:483:LEU:HD11	1.76	0.67
2:F:632:HIS:HA	2:F:635:ARG:HE	1.60	0.67
2:L:613:TYR:CE2	2:L:618:HIS:HE1	2.12	0.67
1:D:874:ILE:HG21	1:D:1000:ARG:HG2	1.76	0.67
2:I:389:PHE:HE1	2:I:493:SER:HB2	1.60	0.67
2:B:489:ASN:ND2	2:B:500:LYS:O	2.27	0.67
1:D:675:ILE:HD13	1:D:739:LEU:HD23	1.77	0.67
1:D:920:LEU:HD23	1:D:933:ARG:HD3	1.76	0.67
2:L:285:PRO:HG2	2:L:294:LEU:HD21	1.75	0.67
2:B:652:THR:OG1	2:B:654:ASP:O	2.13	0.67
2:B:667:LYS:HG3	1:A:378:LEU:HD12	1.77	0.67
2:F:613:TYR:HE1	2:F:618:HIS:HE1	1.41	0.67
2:C:601:SER:OG	2:C:603:SER:O	2.13	0.66
1:D:559:ARG:HH22	1:D:1003:TRP:HE1	1.44	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:573:LEU:HD22	2:F:263:ARG:HG3	1.77	0.66
2:F:623:ASN:OD1	1:D:747:SER:OG	2.11	0.66
2:B:291:TYR:HB3	2:B:313:VAL:HG21	1.78	0.66
2:H:658:CYS:SG	2:H:659:ILE:N	2.67	0.66
2:E:291:TYR:HB3	2:E:313:VAL:HG21	1.78	0.66
2:F:285:PRO:HG3	2:F:366:PHE:CE1	2.29	0.66
2:L:425:ASN:OD1	2:L:447:ASN:ND2	2.29	0.66
1:D:750:ARG:NH1	1:D:843:PRO:O	2.29	0.66
2:E:678:THR:HG22	2:E:679:GLN:H	1.60	0.66
1:A:990:LYS:HE2	1:A:990:LYS:H	1.62	0.65
2:C:504:LEU:HD23	2:C:507:ILE:HD12	1.78	0.65
1:J:704:LYS:HD3	1:J:768:LYS:HA	1.77	0.65
2:L:654:ASP:OD1	2:L:656:LEU:N	2.27	0.65
2:B:449:MET:O	2:B:452:LEU:HG	1.96	0.65
2:F:654:ASP:OD1	2:F:656:LEU:N	2.30	0.65
1:G:439:ARG:HH12	2:I:614:ASP:HB3	1.62	0.65
2:H:440:ARG:HH21	2:H:561:TYR:HE2	1.45	0.65
1:A:417:GLN:N	1:A:419:GLU:OE1	2.28	0.65
1:G:442:ILE:HD11	2:I:619:GLN:HB3	1.79	0.65
1:D:743:ASP:HA	1:D:746:PHE:HD2	1.61	0.65
2:E:278:PRO:HG3	2:E:296:PRO:HD2	1.78	0.65
1:G:507:LEU:HD11	1:G:520:ILE:HD11	1.79	0.65
1:J:945:ILE:HA	1:J:956:PRO:HA	1.79	0.65
2:C:249:ASN:ND2	1:A:389:GLU:O	2.27	0.65
2:E:658:CYS:SG	2:E:659:ILE:N	2.69	0.65
1:G:429:LEU:HB3	2:I:657:ASN:HD22	1.62	0.65
2:E:276:VAL:HG23	2:E:293:ASN:OD1	1.97	0.64
2:C:657:ASN:ND2	1:A:418:ASN:OD1	2.30	0.64
2:I:258:ILE:N	2:I:572:GLU:OE2	2.30	0.64
1:D:597:GLU:OE2	1:D:628:SER:OG	2.12	0.64
2:E:533:ASN:HB3	2:E:536:SER:HA	1.78	0.64
2:H:337:ASN:ND2	1:J:494:PHE:O	2.30	0.64
2:H:327:LEU:HB3	2:H:371:ILE:O	1.98	0.64
2:B:326:ARG:NH2	2:B:368:ASP:OD1	2.30	0.64
2:K:613:TYR:HE1	2:K:617:PHE:CD2	2.16	0.64
1:A:1029:PRO:HG2	1:A:1032:GLN:HG3	1.79	0.63
2:C:357:PHE:HD2	2:C:375:PHE:HE1	1.44	0.63
2:F:258:ILE:N	2:F:572:GLU:OE2	2.31	0.63
2:C:270:ASN:OD1	2:B:570:SER:OG	2.15	0.63
2:F:448:PHE:O	2:F:451:LEU:HG	1.98	0.63
2:K:295:VAL:HG13	2:K:312:LYS:HB3	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:797:THR:HG22	1:G:803:THR:HG22	1.79	0.63
2:K:652:THR:OG1	2:K:654:ASP:O	2.15	0.63
2:B:331:ASP:OD1	2:B:332:LYS:N	2.32	0.63
1:D:758:SER:HB2	1:D:838:LEU:HD21	1.81	0.63
1:A:923:ILE:HD11	1:A:927:GLY:HA2	1.81	0.63
2:C:349:ILE:HG22	2:C:419:GLN:HG3	1.81	0.63
1:D:991:ARG:O	1:D:991:ARG:NH1	2.31	0.63
2:L:258:ILE:N	2:L:572:GLU:OE2	2.30	0.63
2:F:397:ILE:HD11	2:F:486:LEU:HB3	1.81	0.63
1:G:945:ILE:HA	1:G:956:PRO:HA	1.81	0.63
2:C:408:GLN:NE2	2:B:559:GLN:OE1	2.32	0.63
1:A:1009:GLY:HA2	1:A:1032:GLN:HE22	1.63	0.62
1:D:505:SER:OG	1:D:560:SER:O	2.17	0.62
2:L:487:SER:OG	2:L:515:MET:SD	2.51	0.62
2:F:508:THR:O	2:F:511:SER:OG	2.17	0.62
1:J:732:PRO:O	1:J:787:TYR:OH	2.14	0.62
2:I:309:THR:HA	2:I:326:ARG:HG2	1.81	0.62
1:J:1085:LEU:O	1:J:1089:ALA:N	2.32	0.62
2:K:533:ASN:OD1	2:K:534:GLY:N	2.31	0.62
2:L:601:SER:HB3	2:L:607:PHE:HD1	1.63	0.62
2:H:582:VAL:O	2:H:586:ASN:ND2	2.29	0.62
2:I:529:LEU:O	2:I:538:LYS:NZ	2.33	0.62
1:G:710:ASN:HA	1:G:721:THR:HA	1.80	0.62
2:K:570:SER:HA	2:K:573:LEU:HD23	1.82	0.62
1:A:963:VAL:HG23	1:A:983:LEU:HA	1.82	0.61
2:B:606:LYS:O	2:B:609:ILE:HG22	2.00	0.61
1:D:417:GLN:HA	1:D:420:LYS:HB2	1.82	0.61
2:H:412:VAL:HG11	2:H:443:LEU:HD21	1.82	0.61
2:H:397:ILE:HD11	2:H:490:ILE:HB	1.82	0.61
2:F:238:GLN:NE2	2:F:253:ALA:HB3	2.16	0.61
2:H:378:TYR:O	2:H:381:SER:OG	2.13	0.61
1:A:465:GLN:NE2	1:A:498:PRO:O	2.33	0.61
2:F:613:TYR:CE1	2:F:618:HIS:HE1	2.18	0.61
2:I:406:LEU:HG	2:I:483:LEU:HD21	1.81	0.61
1:J:790:ASN:HB3	1:J:851:ILE:HD12	1.81	0.61
1:J:855:ALA:HB1	1:J:859:ARG:HH12	1.65	0.61
2:K:226:HIS:HB2	1:J:369:GLY:HA2	1.82	0.61
1:J:941:ARG:NH1	1:J:961:TYR:OH	2.34	0.61
2:L:238:GLN:HE21	2:L:252:SER:HB2	1.65	0.61
1:J:522:LEU:HD21	1:J:851:ILE:HG12	1.83	0.61
2:L:406:LEU:HD21	2:L:525:VAL:HG11	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:512:ILE:HA	2:H:515:MET:HG3	1.81	0.61
1:J:360:ASP:OD1	1:J:363:TYR:N	2.33	0.61
1:G:497:THR:HG21	2:K:337:ASN:HB3	1.83	0.61
2:I:559:GLN:O	2:I:562:THR:OG1	2.13	0.61
1:G:892:TYR:HA	1:G:956:PRO:HD2	1.83	0.60
2:F:238:GLN:HE22	2:F:253:ALA:HB3	1.66	0.60
2:C:284:ILE:HG13	2:C:285:PRO:HD2	1.83	0.60
1:A:891:GLU:OE2	1:A:990:LYS:NZ	2.34	0.60
2:C:648:LEU:HG	2:C:663:TYR:HE1	1.65	0.60
2:H:295:VAL:HG13	2:H:312:LYS:HB3	1.83	0.60
2:K:330:ILE:HG13	2:K:371:ILE:HG23	1.84	0.60
2:K:341:LYS:HE2	2:K:341:LYS:HA	1.83	0.60
2:C:258:ILE:N	2:C:572:GLU:OE2	2.35	0.60
2:E:388:HIS:HB3	2:E:397:ILE:HD11	1.84	0.60
1:G:497:THR:HB	2:K:341:LYS:HE3	1.83	0.60
2:L:473:GLN:OE1	2:L:538:LYS:N	2.34	0.60
2:C:292:PHE:HE2	2:C:316:ASN:HA	1.67	0.60
1:D:1035:ASP:OD1	1:D:1037:ALA:N	2.34	0.60
2:C:402:LEU:HA	2:C:405:TYR:HD2	1.67	0.59
2:I:305:LEU:HD12	2:I:306:ASN:HB2	1.84	0.59
2:L:631:THR:OG1	1:J:389:GLU:OE1	2.20	0.59
2:C:614:ASP:OD2	2:B:595:ARG:NH2	2.35	0.59
2:F:418:SER:OG	2:F:419:GLN:OE1	2.17	0.59
2:I:323:VAL:HG23	2:I:377:TYR:HA	1.84	0.59
2:C:580:ARG:NH2	1:A:363:TYR:O	2.35	0.59
1:J:391:THR:HG22	1:J:445:TYR:HD1	1.67	0.59
2:H:449:MET:HA	2:H:452:LEU:HG	1.84	0.59
2:K:567:SER:O	2:K:570:SER:OG	2.14	0.59
2:E:378:TYR:O	2:E:381:SER:OG	2.11	0.59
2:C:529:LEU:O	2:C:538:LYS:NZ	2.34	0.59
2:F:301:ASN:HD22	2:F:308:THR:HA	1.68	0.59
2:C:492:ASN:ND2	2:C:498:ALA:O	2.31	0.59
2:K:389:PHE:HE2	2:K:429:TRP:HZ3	1.50	0.59
2:L:584:LYS:HG3	2:L:674:PHE:CD2	2.37	0.59
2:H:678:THR:HG22	2:H:679:GLN:H	1.66	0.59
2:K:423:ILE:N	2:K:475:ASP:OD2	2.35	0.59
1:J:623:ASN:HD22	1:J:849:ILE:HD13	1.67	0.58
2:F:346:TRP:HZ2	2:F:448:PHE:HB3	1.67	0.58
2:I:355:ILE:HD12	2:I:378:TYR:HD2	1.68	0.58
1:G:1025:ASN:O	1:G:1025:ASN:ND2	2.34	0.58
1:J:994:ARG:O	1:J:997:VAL:N	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:854:ASP:HB3	1:A:857:GLU:HB3	1.85	0.58
2:C:643:GLY:O	2:C:644:ILE:HG13	2.02	0.58
2:I:436:GLY:HA3	2:I:440:ARG:CZ	2.33	0.58
2:C:323:VAL:HG23	2:C:377:TYR:HA	1.86	0.58
2:E:399:ASN:ND2	2:E:519:ASP:OD2	2.36	0.58
1:J:909:ILE:HD11	1:J:942:ILE:HD11	1.85	0.58
2:L:652:THR:HG22	2:L:653:PRO:HD2	1.84	0.58
2:E:467:THR:OG1	2:E:468:ILE:N	2.35	0.58
2:F:619:GLN:HB2	2:F:627:ILE:O	2.04	0.58
2:L:654:ASP:OD2	1:J:420:LYS:HG3	2.04	0.58
1:D:522:LEU:HD22	1:D:793:VAL:HG23	1.85	0.58
2:E:429:TRP:HZ3	2:E:485:ASN:HB3	1.69	0.58
2:F:487:SER:OG	2:F:515:MET:SD	2.57	0.58
2:F:529:LEU:O	2:F:538:LYS:NZ	2.37	0.58
2:L:290:ASP:O	2:L:316:ASN:N	2.37	0.58
1:D:750:ARG:NH2	1:D:846:THR:OG1	2.37	0.57
1:G:914:VAL:HG23	1:G:971:TYR:HA	1.86	0.57
2:C:584:LYS:HE3	1:A:359:ASP:HB2	1.86	0.57
1:J:909:ILE:HD12	1:J:944:ILE:HD12	1.87	0.57
1:A:438:MET:HB3	1:A:441:ALA:HB2	1.86	0.57
2:B:601:SER:OG	2:B:602:GLU:N	2.37	0.57
2:F:336:PRO:O	2:F:339:ILE:HG13	2.04	0.57
2:L:623:ASN:OD1	1:J:747:SER:HB2	2.04	0.57
1:J:675:ILE:HD11	1:J:741:LEU:HD21	1.87	0.57
1:G:439:ARG:NH1	2:I:614:ASP:HB3	2.18	0.57
2:I:402:LEU:HA	2:I:405:TYR:HD2	1.69	0.57
1:A:558:GLU:O	1:A:561:HIS:ND1	2.37	0.57
2:E:296:PRO:HA	2:E:311:PHE:HB3	1.87	0.57
2:F:297:LEU:O	2:F:308:THR:HG21	2.05	0.57
2:K:257:PHE:HA	2:K:438:PRO:HB2	1.87	0.57
2:L:601:SER:OG	2:L:603:SER:O	2.22	0.57
2:B:544:THR:HA	2:B:547:PHE:HD2	1.69	0.57
2:E:649:MET:H	1:D:347:PHE:HE2	1.53	0.57
1:D:618:MET:N	1:D:619:PRO:HD2	2.20	0.57
2:L:437:ASP:HB2	2:L:438:PRO:HA	1.86	0.57
1:D:447:CYS:HB3	1:D:450:ASP:HB2	1.87	0.57
2:I:487:SER:OG	2:I:515:MET:SD	2.58	0.57
2:K:584:LYS:NZ	1:J:378:LEU:O	2.24	0.57
1:G:416:SER:HA	1:G:429:LEU:HD23	1.86	0.56
2:I:292:PHE:HE2	2:I:316:ASN:HA	1.70	0.56
2:C:437:ASP:HB2	2:C:438:PRO:HA	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:556:GLU:HG3	2:I:352:THR:OG1	2.05	0.56
2:H:567:SER:O	2:H:570:SER:OG	2.18	0.56
2:K:658:CYS:SG	2:K:659:ILE:N	2.78	0.56
2:B:257:PHE:HA	2:B:438:PRO:HB2	1.87	0.56
1:D:942:ILE:HG13	1:D:998:VAL:HG11	1.87	0.56
1:G:342:ALA:HB1	2:H:620:VAL:O	2.06	0.56
1:A:522:LEU:HD22	1:A:793:VAL:HG23	1.87	0.56
2:C:336:PRO:O	2:C:339:ILE:HG13	2.05	0.56
2:C:406:LEU:HG	2:C:483:LEU:HD21	1.87	0.56
2:I:654:ASP:OD1	2:I:656:LEU:N	2.39	0.56
2:B:403:TRP:CH2	2:B:522:PHE:HB3	2.41	0.56
1:D:546:LEU:HD12	1:D:629:GLN:HG2	1.88	0.56
2:F:652:THR:OG1	2:F:654:ASP:OD1	2.23	0.56
2:L:635:ARG:NH1	1:J:389:GLU:OE1	2.35	0.56
2:L:424:GLY:HA3	2:L:447:ASN:HB3	1.86	0.56
2:L:297:LEU:O	2:L:308:THR:HG21	2.05	0.56
2:E:423:ILE:N	2:E:475:ASP:OD2	2.38	0.56
2:F:258:ILE:HG13	2:F:259:PRO:HD2	1.87	0.56
2:I:291:TYR:HB3	2:I:313:VAL:HG11	1.88	0.56
1:A:513:ASN:OD1	1:A:571:GLN:NE2	2.38	0.56
2:B:423:ILE:N	2:B:475:ASP:OD2	2.35	0.56
1:G:1015:HIS:H	1:G:1015:HIS:CD2	2.22	0.56
1:G:477:PRO:O	1:G:480:SER:OG	2.18	0.56
2:L:357:PHE:HZ	2:L:360:ILE:HB	1.71	0.56
1:A:746:PHE:O	1:A:749:ILE:HG13	2.06	0.56
2:B:466:SER:OG	2:B:467:THR:N	2.38	0.56
2:E:276:VAL:HG12	2:F:644:ILE:HG12	1.86	0.56
2:H:417:HIS:CE1	2:H:472:GLN:HG3	2.41	0.56
2:H:427:LEU:HB2	2:H:478:TYR:HB3	1.88	0.56
2:L:563:GLU:OE2	2:K:442:LYS:NZ	2.34	0.56
1:A:631:ILE:O	1:A:634:GLU:HG2	2.06	0.56
1:G:482:LEU:HD21	1:G:828:LEU:HB2	1.87	0.56
2:B:615:TYR:OH	1:A:345:ASP:OD2	2.13	0.55
2:H:533:ASN:OD1	2:H:534:GLY:N	2.39	0.55
1:G:522:LEU:HD22	1:G:793:VAL:HG23	1.87	0.55
2:K:621:ASP:N	2:K:625:LYS:O	2.36	0.55
2:L:429:TRP:HZ2	2:L:485:ASN:HB3	1.71	0.55
1:A:892:TYR:HA	1:A:956:PRO:HG2	1.89	0.55
2:K:617:PHE:HE1	2:K:633:VAL:HG13	1.71	0.55
2:B:429:TRP:HA	2:B:432:VAL:HG12	1.89	0.55
2:F:301:ASN:OD1	2:F:303:ASP:N	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:423:ILE:HG21	2:I:475:ASP:HB3	1.87	0.55
1:A:546:LEU:HD12	1:A:629:GLN:HG2	1.89	0.55
1:D:507:LEU:HD21	1:D:557:MET:SD	2.47	0.55
2:E:353:ASN:ND2	2:E:411:ASN:HD22	2.04	0.55
1:J:968:ILE:HG13	1:J:971:TYR:CZ	2.41	0.55
2:B:619:GLN:NE2	1:A:343:TYR:HB2	2.22	0.55
2:B:582:VAL:O	2:B:586:ASN:ND2	2.34	0.55
1:A:523:TYR:OH	1:A:623:ASN:OD1	2.23	0.55
2:I:574:GLU:OE2	2:I:638:ASN:ND2	2.39	0.55
1:A:1035:ASP:OD1	1:A:1036:THR:N	2.41	0.54
2:C:358:ARG:O	2:C:374:VAL:HB	2.07	0.54
2:I:291:TYR:HB3	2:I:313:VAL:CG1	2.37	0.54
2:H:403:TRP:CE3	2:H:550:LYS:HG3	2.41	0.54
2:K:577:ARG:HA	2:K:580:ARG:HE	1.71	0.54
2:L:274:LEU:HD11	2:K:229:ALA:HA	1.89	0.54
2:B:567:SER:O	2:B:570:SER:HB3	2.08	0.54
2:K:352:THR:O	2:K:442:LYS:NZ	2.29	0.54
2:F:357:PHE:HD1	2:F:375:PHE:HE1	1.53	0.54
1:G:760:PHE:CE1	1:G:771:LEU:HD23	2.42	0.54
2:B:327:LEU:HB2	2:B:371:ILE:O	2.06	0.54
1:D:1032:GLN:OE1	1:D:1032:GLN:N	2.40	0.54
2:E:257:PHE:HA	2:E:438:PRO:HB2	1.88	0.54
2:H:619:GLN:O	2:H:626:PRO:HA	2.07	0.54
2:I:492:ASN:O	2:I:497:THR:N	2.37	0.54
2:L:429:TRP:HE1	2:L:485:ASN:HB2	1.73	0.54
2:B:644:ILE:O	2:B:663:TYR:HB2	2.08	0.54
2:C:542:ASP:O	2:C:546:HIS:ND1	2.33	0.54
2:L:391:ASN:OD1	2:L:392:PHE:N	2.39	0.54
1:J:944:ILE:HG12	1:J:957:PHE:CZ	2.43	0.54
2:L:586:ASN:ND2	2:K:613:TYR:OH	2.41	0.54
2:B:289:GLN:HG2	2:B:361:PHE:CG	2.43	0.54
2:C:280:SER:HB3	2:C:283:VAL:HG22	1.90	0.54
2:H:385:TYR:HB2	2:H:429:TRP:HD1	1.73	0.54
2:I:327:LEU:HB2	2:I:371:ILE:O	2.08	0.54
2:K:511:SER:HA	2:K:514:ASP:HB2	1.89	0.54
2:L:621:ASP:OD1	2:L:622:SER:N	2.41	0.54
2:B:406:LEU:HG	2:B:547:PHE:CZ	2.43	0.53
1:D:992:LEU:HD23	1:D:997:VAL:HG11	1.90	0.53
2:E:417:HIS:CE1	2:E:472:GLN:HG3	2.42	0.53
2:F:653:PRO:HA	1:D:439:ARG:HE	1.74	0.53
2:E:615:TYR:HD1	1:D:341:LEU:HD13	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:962:VAL:HG21	1:A:994:ARG:HB2	1.89	0.53
1:G:940:ALA:O	1:G:962:VAL:HG12	2.08	0.53
2:H:614:ASP:OD2	2:I:595:ARG:NH2	2.38	0.53
2:I:652:THR:OG1	2:I:654:ASP:OD1	2.24	0.53
1:J:1030:ARG:O	1:J:1033:ILE:HG12	2.07	0.53
2:C:290:ASP:O	2:C:316:ASN:N	2.38	0.53
2:H:296:PRO:HA	2:H:311:PHE:HD1	1.73	0.53
2:L:353:ASN:O	2:L:442:LYS:HA	2.09	0.53
2:L:449:MET:HA	2:L:452:LEU:HD12	1.91	0.53
1:A:477:PRO:O	1:A:480:SER:OG	2.19	0.53
2:K:425:ASN:ND2	2:K:425:ASN:O	2.42	0.53
2:B:508:THR:OG1	2:B:511:SER:HB3	2.09	0.53
2:I:385:TYR:HB2	2:I:429:TRP:HB3	1.90	0.53
1:J:1067:ASP:OD1	1:J:1068:SER:N	2.41	0.53
2:K:259:PRO:HB3	2:K:438:PRO:HD3	1.91	0.53
1:A:511:VAL:O	1:A:936:ARG:NH2	2.42	0.53
2:E:357:PHE:CE1	2:E:360:ILE:HG13	2.43	0.53
1:A:966:ASN:OD1	1:A:967:HIS:N	2.38	0.53
2:K:287:ILE:HG22	2:K:292:PHE:HB3	1.91	0.53
2:L:258:ILE:HG13	2:L:259:PRO:HD2	1.91	0.53
2:E:591:ARG:HA	2:F:618:HIS:HD2	1.73	0.53
2:F:295:VAL:HG13	2:F:312:LYS:HB3	1.90	0.53
2:E:591:ARG:HA	2:F:618:HIS:CD2	2.44	0.53
1:G:855:ALA:HB1	1:G:859:ARG:HH12	1.74	0.53
2:I:383:SER:O	2:I:387:TYR:N	2.40	0.53
2:L:248:PRO:HG3	2:K:317:TYR:CZ	2.44	0.53
2:E:437:ASP:N	2:E:438:PRO:HD2	2.23	0.53
2:F:338:LYS:O	2:F:342:ILE:HG12	2.09	0.53
2:I:578:LEU:HD22	2:I:637:LEU:HB3	1.91	0.53
1:J:514:HIS:O	1:J:517:ASN:ND2	2.29	0.53
1:J:988:SER:O	1:J:989:THR:OG1	2.26	0.53
2:L:444:SER:HG	2:L:445:HIS:CE1	2.27	0.53
2:B:572:GLU:OE2	2:B:575:ASN:ND2	2.41	0.52
2:E:349:ILE:HD11	2:E:421:LEU:HD12	1.91	0.52
2:E:404:ILE:HG22	2:E:408:GLN:HE21	1.75	0.52
2:L:545:SER:HA	2:L:548:TYR:CE2	2.43	0.52
1:D:631:ILE:O	1:D:634:GLU:HG2	2.09	0.52
1:D:836:GLU:HA	1:D:839:LYS:HE3	1.92	0.52
2:K:426:THR:HG21	2:K:444:SER:O	2.10	0.52
2:B:378:TYR:O	2:B:381:SER:OG	2.14	0.52
2:B:325:LYS:HD3	2:B:445:HIS:HE1	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:607:PHE:O	2:F:610:ILE:HG13	2.09	0.52
1:A:996:ASN:O	1:A:1000:ARG:HB2	2.09	0.52
1:D:957:PHE:HD1	1:D:958:VAL:HG22	1.74	0.52
2:H:426:THR:HG21	2:H:446:CYS:HA	1.91	0.52
2:I:238:GLN:OE1	2:I:238:GLN:N	2.37	0.52
2:I:601:SER:OG	2:I:603:SER:O	2.27	0.52
2:L:442:LYS:NZ	2:K:563:GLU:OE2	2.39	0.52
2:L:435:THR:HG22	2:L:436:GLY:H	1.73	0.52
2:L:569:LEU:HD11	2:K:568:VAL:HG13	1.91	0.52
2:C:435:THR:HG22	2:C:436:GLY:H	1.74	0.52
2:C:578:LEU:O	2:C:582:VAL:HG23	2.10	0.52
2:F:606:LYS:O	2:F:609:ILE:HG12	2.09	0.52
1:G:1025:ASN:C	1:G:1025:ASN:HD22	2.13	0.52
1:G:878:ASP:HB2	1:G:894:LEU:HD21	1.91	0.52
2:H:405:TYR:HA	2:H:441:ILE:HD13	1.92	0.52
1:J:698:TYR:HE2	1:J:755:TRP:HE1	1.56	0.52
2:K:510:GLN:NE2	2:K:514:ASP:OD1	2.42	0.52
2:C:291:TYR:HB3	2:C:313:VAL:CG2	2.40	0.52
2:F:409:LEU:HD11	2:F:441:ILE:HG21	1.92	0.52
2:H:484:PHE:CE1	2:H:488:ILE:HG13	2.45	0.52
2:K:391:ASN:OD1	2:K:392:PHE:N	2.43	0.52
2:K:425:ASN:HB3	2:K:478:TYR:CZ	2.44	0.52
2:B:392:PHE:CD1	2:B:393:PRO:HA	2.44	0.52
2:C:573:LEU:HD23	2:B:572:GLU:HG2	1.91	0.52
2:H:429:TRP:HZ3	2:H:485:ASN:ND2	2.07	0.52
2:H:595:ARG:HD3	2:I:600:TRP:CD1	2.44	0.52
2:B:401:TYR:HD1	2:B:404:ILE:HD12	1.75	0.52
2:C:386:ASP:HA	2:C:390:VAL:HB	1.92	0.52
2:E:583:ASN:ND2	2:F:628:MET:SD	2.82	0.52
2:K:437:ASP:N	2:K:438:PRO:HD2	2.25	0.52
2:L:280:SER:HB2	2:L:283:VAL:HG22	1.91	0.52
2:C:591:ARG:O	2:C:594:SER:OG	2.22	0.52
2:F:435:THR:HG22	2:F:436:GLY:H	1.74	0.52
2:F:590:GLY:O	2:F:595:ARG:NH1	2.43	0.52
2:I:297:LEU:O	2:I:308:THR:HG21	2.10	0.52
2:E:620:VAL:O	1:D:342:ALA:HB1	2.10	0.51
1:D:910:ASP:OD1	1:D:911:ALA:N	2.42	0.51
2:H:386:ASP:HA	2:H:390:VAL:HG12	1.92	0.51
2:H:581:LEU:HD23	2:H:637:LEU:HB3	1.92	0.51
2:E:386:ASP:HA	2:E:390:VAL:HB	1.91	0.51
2:C:540:ILE:HG23	2:B:548:TYR:OH	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:258:ILE:HG13	2:I:259:PRO:HD2	1.92	0.51
2:K:278:PRO:HD3	2:K:295:VAL:HB	1.92	0.51
2:L:334:MET:HB2	2:L:338:LYS:HE3	1.91	0.51
2:F:631:THR:O	2:F:635:ARG:HG3	2.11	0.51
2:H:592:ILE:HD12	2:I:653:PRO:HB3	1.91	0.51
2:I:413:ILE:O	2:I:416:ILE:HG13	2.11	0.51
2:L:437:ASP:OD1	2:L:437:ASP:N	2.42	0.51
2:E:386:ASP:HB3	2:E:391:ASN:OD1	2.10	0.51
2:H:548:TYR:OH	2:I:545:SER:OG	2.25	0.51
2:I:263:ARG:NH1	2:I:264:GLU:HG3	2.25	0.51
2:I:619:GLN:HB2	2:I:627:ILE:O	2.11	0.51
2:L:301:ASN:ND2	2:L:308:THR:HA	2.25	0.51
2:L:429:TRP:CZ2	2:L:485:ASN:HB3	2.45	0.51
2:C:399:ASN:OD1	2:C:400:ASN:N	2.43	0.51
1:D:854:ASP:HB3	1:D:857:GLU:HB3	1.92	0.51
2:E:449:MET:HA	2:E:452:LEU:HD12	1.91	0.51
2:F:437:ASP:HA	2:F:438:PRO:C	2.31	0.51
2:C:569:LEU:HD11	2:B:568:VAL:HG13	1.93	0.51
2:H:407:VAL:HG11	2:H:554:VAL:HG11	1.93	0.51
2:H:607:PHE:N	2:H:608:PRO:HD2	2.26	0.51
2:I:321:ALA:O	2:I:322:TYR:CG	2.64	0.51
2:L:287:ILE:HG13	2:L:292:PHE:HB3	1.93	0.51
1:D:677:GLY:O	1:D:678:ILE:HG13	2.11	0.51
1:D:893:LYS:O	1:D:946:ARG:NH2	2.38	0.51
1:G:1003:TRP:O	1:G:1006:MET:HG3	2.11	0.51
2:B:407:VAL:O	2:B:410:THR:OG1	2.23	0.51
2:C:247:LYS:HB3	2:C:248:PRO:HD2	1.92	0.51
1:D:556:MET:HE1	1:D:1025:ASN:O	2.09	0.51
1:J:1015:HIS:HD1	1:J:1036:THR:HG1	1.55	0.51
1:J:482:LEU:HD21	1:J:828:LEU:HB2	1.92	0.51
2:C:657:ASN:HD21	1:A:415:SER:HB2	1.76	0.50
2:B:525:VAL:O	2:B:528:TYR:HB3	2.11	0.50
2:C:584:LYS:HG2	2:C:674:PHE:CE2	2.47	0.50
1:G:758:SER:HB2	1:G:838:LEU:HD21	1.93	0.50
1:G:799:ASN:OD1	1:G:799:ASN:N	2.44	0.50
2:H:543:LEU:O	2:H:546:HIS:HB2	2.10	0.50
2:H:274:LEU:HD21	2:I:639:LYS:HA	1.93	0.50
2:K:627:ILE:HD11	1:J:343:TYR:CG	2.45	0.50
2:C:352:THR:OG1	2:B:556:GLU:HG2	2.12	0.50
2:B:575:ASN:HB3	1:A:365:LEU:HD12	1.92	0.50
2:H:343:TYR:HA	2:H:357:PHE:HE2	1.75	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:540:ILE:HD12	2:L:540:ILE:H	1.77	0.50
2:B:518:ILE:HG22	2:B:520:ASP:N	2.21	0.50
2:E:429:TRP:CD1	2:E:430:ARG:N	2.79	0.50
2:F:309:THR:O	2:F:326:ARG:HB3	2.11	0.50
1:A:952:LEU:O	1:A:955:VAL:HG12	2.11	0.50
1:A:988:SER:O	1:A:989:THR:OG1	2.29	0.50
2:E:613:TYR:OH	2:F:586:ASN:ND2	2.43	0.50
1:J:477:PRO:O	1:J:480:SER:OG	2.20	0.50
2:C:586:ASN:ND2	2:B:586:ASN:OD1	2.45	0.50
2:H:318:ASP:HB3	2:H:320:LYS:HB2	1.94	0.50
2:H:341:LYS:HA	1:J:497:THR:HG21	1.92	0.50
1:J:853:CYS:SG	1:J:854:ASP:N	2.84	0.50
2:K:389:PHE:HE1	2:K:493:SER:HB3	1.76	0.50
2:E:357:PHE:HE1	2:E:360:ILE:HG13	1.76	0.50
2:H:402:LEU:HD11	2:H:487:SER:HB3	1.94	0.50
1:D:528:GLU:HG3	1:D:857:GLU:OE2	2.11	0.50
1:D:945:ILE:HG23	1:D:956:PRO:HA	1.93	0.50
2:E:563:GLU:OE2	2:F:442:LYS:NZ	2.37	0.50
2:L:574:GLU:HG2	2:L:578:LEU:HD13	1.92	0.50
1:A:997:VAL:HG23	1:A:998:VAL:N	2.26	0.50
2:C:603:SER:OG	2:C:604:GLY:N	2.44	0.50
1:D:1015:HIS:HD1	1:D:1036:THR:HG1	1.54	0.50
2:E:592:ILE:HD12	2:F:653:PRO:HB3	1.94	0.50
2:I:397:ILE:HD11	2:I:402:LEU:HD21	1.93	0.50
2:B:389:PHE:CD2	2:B:499:PRO:HG3	2.46	0.50
2:F:649:MET:HG2	1:D:435:LYS:HE2	1.94	0.50
1:J:507:LEU:HD21	1:J:557:MET:SD	2.52	0.50
1:A:701:TYR:O	1:A:705:ASN:HB3	2.12	0.49
2:B:331:ASP:OD1	2:B:332:LYS:HG2	2.12	0.49
2:B:667:LYS:HG3	1:A:378:LEU:HB2	1.94	0.49
2:C:238:GLN:NE2	2:C:253:ALA:HB3	2.27	0.49
2:F:280:SER:HB2	2:F:283:VAL:HG22	1.94	0.49
2:H:265:ASP:O	2:H:269:LYS:HG3	2.12	0.49
1:J:1000:ARG:HE	1:J:1004:LEU:HD11	1.77	0.49
1:J:467:TYR:HD2	1:J:836:GLU:HG2	1.76	0.49
1:J:505:SER:OG	1:J:561:HIS:O	2.18	0.49
2:L:238:GLN:HE22	2:L:254:ASP:H	1.60	0.49
2:C:579:PHE:HE1	2:B:582:VAL:HG21	1.77	0.49
2:E:607:PHE:N	2:E:608:PRO:HD2	2.27	0.49
1:G:764:ILE:HG22	1:G:769:ALA:HA	1.94	0.49
2:I:306:ASN:OD1	2:I:307:LYS:N	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:387:TYR:CE2	2:L:434:ILE:HD12	2.48	0.49
2:F:397:ILE:HG23	2:F:490:ILE:HG13	1.93	0.49
1:G:373:TYR:HE1	2:I:233:LEU:HB2	1.77	0.49
2:F:349:ILE:HG22	2:F:419:GLN:HE21	1.77	0.49
1:G:546:LEU:HD12	1:G:629:GLN:HG2	1.95	0.49
1:G:761:TYR:CE1	1:G:786:LYS:HG3	2.48	0.49
2:H:273:ILE:HD11	2:H:379:PRO:HG3	1.94	0.49
2:I:558:SER:O	2:I:562:THR:HG23	2.13	0.49
2:L:677:ILE:O	2:K:626:PRO:HG2	2.13	0.49
1:A:695:ILE:O	1:A:698:TYR:HB2	2.13	0.49
1:G:925:HIS:O	1:G:926:GLN:HG2	2.12	0.49
1:J:1033:ILE:HG13	1:J:1034:ARG:N	2.28	0.49
2:L:675:ARG:O	2:L:679:GLN:HG2	2.12	0.49
1:A:467:TYR:CD2	1:A:836:GLU:HG2	2.48	0.49
1:A:855:ALA:HB1	1:A:859:ARG:HH12	1.77	0.49
2:B:362:GLN:HB3	1:A:923:ILE:HG23	1.94	0.49
2:C:555:LEU:HD11	2:B:554:VAL:HG13	1.93	0.49
2:F:292:PHE:CE2	2:F:316:ASN:HA	2.48	0.49
1:G:796:ILE:HG23	1:G:844:TRP:HD1	1.77	0.49
2:H:509:PRO:O	2:H:512:ILE:HG13	2.13	0.49
1:J:942:ILE:HG21	1:J:998:VAL:CG1	2.42	0.49
2:K:577:ARG:HH21	2:K:578:LEU:HD11	1.77	0.49
2:I:295:VAL:HG13	2:I:312:LYS:HB3	1.94	0.49
2:I:533:ASN:ND2	2:I:536:SER:O	2.46	0.49
1:A:1019:ASN:O	1:A:1023:HIS:ND1	2.46	0.49
1:A:962:VAL:CG2	1:A:994:ARG:HB2	2.42	0.49
2:C:318:ASP:OD2	2:C:322:TYR:OH	2.24	0.49
1:G:620:GLN:NE2	1:G:848:GLU:OE1	2.46	0.49
1:G:796:ILE:HG23	1:G:844:TRP:CD1	2.47	0.49
2:L:483:LEU:HD23	2:L:522:PHE:CE1	2.48	0.49
1:A:641:ASN:O	1:A:642:ILE:HG13	2.13	0.49
2:C:238:GLN:OE1	2:C:243:LYS:NZ	2.46	0.49
2:C:295:VAL:HG13	2:C:312:LYS:HB3	1.95	0.49
2:H:405:TYR:HD1	2:H:441:ILE:HD11	1.78	0.49
1:G:756:LEU:HD21	1:G:789:LEU:HD22	1.94	0.49
2:K:252:SER:HB2	2:K:255:GLN:HB2	1.95	0.49
2:L:587:CYS:HB2	2:K:628:MET:SD	2.52	0.49
2:L:629:ASP:OD1	2:L:631:THR:HG22	2.12	0.49
2:C:437:ASP:OD1	2:C:437:ASP:N	2.44	0.48
2:E:577:ARG:HA	2:E:580:ARG:HE	1.79	0.48
2:F:312:LYS:HG3	2:F:377:TYR:HE2	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:458:ASP:CB	1:J:1030:ARG:H	2.26	0.48
2:I:549:ASP:N	2:I:549:ASP:OD1	2.46	0.48
1:A:853:CYS:SG	1:A:854:ASP:N	2.86	0.48
2:B:325:LYS:HD3	2:B:445:HIS:CE1	2.48	0.48
2:B:437:ASP:N	2:B:438:PRO:HD2	2.28	0.48
2:C:582:VAL:O	2:C:586:ASN:HB2	2.12	0.48
2:C:631:THR:O	2:C:635:ARG:HG3	2.13	0.48
2:F:601:SER:OG	2:F:603:SER:O	2.29	0.48
1:J:559:ARG:O	1:J:561:HIS:ND1	2.45	0.48
2:K:349:ILE:HD11	2:K:421:LEU:HD12	1.94	0.48
2:L:579:PHE:CE1	2:K:578:LEU:HB3	2.48	0.48
2:L:301:ASN:OD1	2:L:303:ASP:N	2.46	0.48
2:B:507:ILE:O	2:B:509:PRO:HD3	2.13	0.48
2:F:397:ILE:HG21	2:F:490:ILE:HA	1.96	0.48
1:J:631:ILE:O	1:J:634:GLU:HG2	2.13	0.48
2:C:353:ASN:H	2:C:442:LYS:NZ	2.12	0.48
2:C:576:GLY:O	2:C:579:PHE:HB3	2.14	0.48
1:D:432:ASP:OD1	1:D:433:ARG:N	2.47	0.48
2:E:429:TRP:CZ3	2:E:485:ASN:HB3	2.47	0.48
2:B:264:GLU:N	2:B:264:GLU:OE2	2.45	0.48
1:D:537:LEU:O	1:D:1000:ARG:NH1	2.44	0.48
2:E:612:PHE:HE2	2:E:640:LEU:HD22	1.79	0.48
2:F:429:TRP:CZ2	2:F:485:ASN:HB3	2.49	0.48
2:H:359:ASP:H	2:H:374:VAL:HG12	1.79	0.48
2:L:590:GLY:O	2:L:595:ARG:NH1	2.46	0.48
1:A:676:SER:OG	1:A:677:GLY:N	2.46	0.48
1:G:653:GLU:O	1:G:726:CYS:HA	2.13	0.48
1:G:824:PHE:CE1	1:G:829:VAL:HG13	2.49	0.48
1:G:910:ASP:OD1	1:G:911:ALA:N	2.45	0.48
2:I:513:ASP:HA	2:I:523:LYS:HD3	1.96	0.48
2:I:631:THR:O	2:I:635:ARG:HG3	2.13	0.48
2:L:355:ILE:HG23	2:L:376:ASP:HB2	1.94	0.48
1:A:765:ILE:HD12	1:A:766:LYS:HG3	1.94	0.48
2:B:616:VAL:HA	2:B:632:HIS:HE1	1.79	0.48
1:D:447:CYS:O	1:D:451:ILE:N	2.47	0.48
2:E:567:SER:O	2:E:570:SER:OG	2.24	0.48
2:F:597:ASP:HB3	2:F:599:ASN:O	2.12	0.48
2:F:603:SER:OG	2:F:604:GLY:N	2.47	0.48
1:G:348:ASN:OD1	2:H:639:LYS:NZ	2.31	0.48
1:J:454:GLN:C	1:J:456:THR:H	2.17	0.48
1:J:537:LEU:HD21	1:J:552:TYR:HE1	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:477:LYS:O	2:C:504:LEU:HD21	2.12	0.48
1:D:895:LEU:HD21	1:D:957:PHE:CE2	2.48	0.48
2:F:581:LEU:HD21	2:F:640:LEU:HD22	1.96	0.48
1:G:853:CYS:SG	1:G:854:ASP:N	2.87	0.48
2:I:406:LEU:HD12	2:I:522:PHE:CE1	2.48	0.48
2:K:248:PRO:HD2	2:K:251:ARG:HE	1.79	0.48
2:L:323:VAL:HG23	2:L:377:TYR:HA	1.95	0.48
2:E:277:PHE:CD2	2:E:278:PRO:HD3	2.48	0.48
2:F:540:ILE:HD12	2:F:540:ILE:H	1.78	0.48
1:J:624:ARG:NH1	1:J:738:GLU:OE1	2.47	0.48
2:L:270:ASN:HD21	2:K:570:SER:HB2	1.78	0.48
2:L:553:MET:O	2:L:556:GLU:HB2	2.13	0.48
2:L:603:SER:OG	2:L:604:GLY:N	2.47	0.48
2:C:620:VAL:O	1:A:441:ALA:HA	2.14	0.48
2:B:599:ASN:N	2:B:599:ASN:OD1	2.40	0.48
2:H:619:GLN:HB2	2:H:627:ILE:O	2.14	0.48
2:H:568:VAL:HG13	2:I:569:LEU:HD11	1.96	0.48
2:K:353:ASN:HB2	2:K:412:VAL:HG13	1.96	0.48
2:L:409:LEU:HA	2:L:412:VAL:HG22	1.95	0.48
1:A:993:VAL:HG22	1:A:995:ARG:H	1.79	0.47
2:B:607:PHE:CE2	2:B:611:LEU:HD11	2.48	0.47
2:F:416:ILE:HG13	2:F:423:ILE:HD13	1.95	0.47
1:G:999:TYR:CE1	1:G:1026:ILE:HB	2.49	0.47
1:J:696:LEU:HB2	1:J:697:PRO:HD3	1.96	0.47
2:K:285:PRO:HG3	2:K:366:PHE:HE1	1.79	0.47
2:L:606:LYS:O	2:L:609:ILE:HG13	2.13	0.47
1:A:696:LEU:HB2	1:A:697:PRO:HD3	1.96	0.47
2:B:495:ASN:OD1	2:B:496:ASN:N	2.45	0.47
1:G:789:LEU:HD23	1:G:821:TRP:HH2	1.80	0.47
2:I:475:ASP:OD1	2:I:476:TYR:N	2.47	0.47
2:I:581:LEU:HD21	2:I:640:LEU:HD22	1.96	0.47
1:J:467:TYR:CD2	1:J:836:GLU:HG2	2.48	0.47
2:L:432:VAL:HG22	2:L:443:LEU:HD13	1.96	0.47
1:A:1048:SER:HB2	1:A:1051:TYR:HB2	1.96	0.47
1:D:456:THR:OG1	1:D:457:SER:N	2.47	0.47
1:G:1020:ASP:O	1:G:1024:ILE:HG13	2.13	0.47
1:G:1069:ILE:HD12	1:G:1069:ILE:H	1.79	0.47
1:G:631:ILE:O	1:G:634:GLU:HG2	2.13	0.47
1:G:888:ALA:HA	1:G:989:THR:HA	1.96	0.47
2:H:587:CYS:HB2	2:I:628:MET:SD	2.55	0.47
2:K:326:ARG:NH2	2:K:368:ASP:OD2	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:566:GLU:OE2	2:K:440:ARG:NH2	2.46	0.47
2:B:291:TYR:HB3	2:B:313:VAL:CG2	2.43	0.47
2:F:578:LEU:O	2:F:582:VAL:HG23	2.14	0.47
1:G:899:GLU:H	1:G:899:GLU:CD	2.18	0.47
2:H:562:THR:OG1	2:I:562:THR:HG22	2.15	0.47
2:B:423:ILE:HG23	2:B:446:CYS:SG	2.54	0.47
2:B:410:THR:HG21	2:B:547:PHE:CE2	2.49	0.47
2:F:654:ASP:OD1	2:F:655:GLU:N	2.47	0.47
2:K:312:LYS:HD2	2:K:377:TYR:CE2	2.50	0.47
2:L:475:ASP:OD1	2:L:476:TYR:N	2.47	0.47
2:C:589:PHE:O	2:B:618:HIS:NE2	2.48	0.47
2:E:618:HIS:CD2	2:F:591:ARG:HD2	2.50	0.47
1:G:503:GLU:HG2	1:G:504:TYR:CD1	2.50	0.47
2:K:246:LEU:O	2:K:248:PRO:HD3	2.13	0.47
2:K:584:LYS:HG3	1:J:381:TRP:CZ3	2.50	0.47
2:L:401:TYR:HA	2:L:404:ILE:HD12	1.96	0.47
2:C:579:PHE:CE1	2:B:582:VAL:HG21	2.49	0.47
2:C:652:THR:HG22	2:C:653:PRO:HD2	1.96	0.47
2:F:291:TYR:HB3	2:F:313:VAL:CG1	2.45	0.47
1:G:955:VAL:HA	1:G:956:PRO:HD3	1.77	0.47
2:H:463:SER:HB3	1:J:1007:GLN:O	2.14	0.47
2:I:338:LYS:O	2:I:342:ILE:HG13	2.15	0.47
2:K:589:PHE:CG	2:K:613:TYR:HD2	2.33	0.47
2:L:234:TYR:CZ	2:K:577:ARG:HD3	2.49	0.47
2:B:280:SER:OG	2:B:284:ILE:O	2.24	0.47
2:B:318:ASP:OD2	2:B:322:TYR:OH	2.25	0.47
2:B:323:VAL:O	2:B:374:VAL:HA	2.14	0.47
2:B:652:THR:HG21	2:B:657:ASN:HB2	1.96	0.47
2:C:578:LEU:HD21	2:C:638:ASN:HA	1.97	0.47
1:D:485:THR:HG22	1:D:486:SER:H	1.78	0.47
2:I:355:ILE:HG12	2:I:444:SER:HA	1.97	0.47
2:I:611:LEU:HD21	2:I:651:VAL:O	2.15	0.47
1:A:698:TYR:HE2	1:A:755:TRP:HE1	1.61	0.47
2:C:406:LEU:HD11	2:C:525:VAL:HG11	1.96	0.47
2:H:383:SER:HA	2:H:433:LEU:HA	1.96	0.47
1:G:365:LEU:HD23	2:H:578:LEU:HD22	1.97	0.47
2:H:628:MET:SD	2:I:583:ASN:ND2	2.88	0.47
1:J:424:GLN:HG3	1:J:425:GLU:H	1.78	0.47
2:C:623:ASN:HA	1:A:743:ASP:HB3	1.96	0.47
2:B:401:TYR:HA	2:B:404:ILE:HD12	1.97	0.47
2:C:483:LEU:HD23	2:C:522:PHE:CE1	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:406:LEU:CD1	2:E:483:LEU:HD11	2.44	0.47
2:L:549:ASP:OD1	2:L:549:ASP:N	2.48	0.47
2:L:631:THR:OG1	2:L:635:ARG:NH1	2.48	0.47
1:A:507:LEU:HD21	1:A:557:MET:SD	2.55	0.47
1:A:624:ARG:NH1	1:A:738:GLU:OE1	2.48	0.47
1:D:418:ASN:C	1:D:420:LYS:H	2.18	0.47
1:D:438:MET:HE1	1:D:743:ASP:H	1.80	0.47
2:H:259:PRO:HB3	2:H:438:PRO:HD3	1.96	0.47
1:J:940:ALA:O	1:J:962:VAL:HG12	2.14	0.47
2:B:469:GLU:O	2:B:473:GLN:HG2	2.15	0.46
2:L:631:THR:O	2:L:635:ARG:HG3	2.15	0.46
1:A:467:TYR:HD2	1:A:836:GLU:HG2	1.79	0.46
2:C:301:ASN:ND2	2:C:303:ASP:O	2.48	0.46
1:G:525:PHE:CE1	1:G:824:PHE:HE2	2.33	0.46
2:H:408:GLN:CD	2:H:441:ILE:HD12	2.35	0.46
2:I:261:ASN:OD1	2:I:262:ILE:N	2.49	0.46
2:L:247:LYS:HB2	2:L:248:PRO:HD2	1.98	0.46
2:C:427:LEU:O	2:C:482:LEU:HD12	2.15	0.46
2:F:353:ASN:O	2:F:442:LYS:HA	2.15	0.46
1:G:896:THR:HG22	1:G:897:HIS:H	1.80	0.46
2:H:570:SER:HA	2:H:573:LEU:HD23	1.97	0.46
2:I:326:ARG:HB2	2:I:366:PHE:HE2	1.79	0.46
2:I:640:LEU:HA	2:I:663:TYR:HD2	1.79	0.46
1:J:908:ALA:O	1:J:944:ILE:HG13	2.15	0.46
2:K:322:TYR:CE1	2:K:358:ARG:HD2	2.50	0.46
2:B:401:TYR:O	2:B:405:TYR:HD1	1.98	0.46
2:C:475:ASP:OD1	2:C:476:TYR:N	2.48	0.46
2:C:607:PHE:HB3	2:C:608:PRO:HD3	1.97	0.46
1:D:1020:ASP:O	1:D:1024:ILE:HG13	2.15	0.46
2:F:406:LEU:HG	2:F:483:LEU:HD11	1.96	0.46
2:K:619:GLN:O	2:K:626:PRO:HA	2.16	0.46
2:L:556:GLU:OE2	2:K:411:ASN:ND2	2.24	0.46
2:C:639:LYS:NZ	2:C:663:TYR:OH	2.48	0.46
2:E:413:ILE:HD13	2:E:423:ILE:HD12	1.98	0.46
2:F:429:TRP:HZ2	2:F:485:ASN:HB3	1.80	0.46
2:I:355:ILE:HD12	2:I:378:TYR:CD2	2.49	0.46
1:A:939:LEU:HG	1:A:962:VAL:HG11	1.98	0.46
2:E:569:LEU:HB2	2:F:569:LEU:HD13	1.96	0.46
2:I:254:ASP:OD1	2:I:254:ASP:N	2.49	0.46
2:I:473:GLN:NE2	2:I:533:ASN:OD1	2.38	0.46
2:L:408:GLN:NE2	2:L:439:GLY:O	2.39	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:561:TYR:HD1	2:L:564:TYR:HB3	1.81	0.46
2:B:450:ASP:OD1	2:B:454:ASN:ND2	2.48	0.46
2:C:258:ILE:HG13	2:C:259:PRO:HD2	1.97	0.46
1:D:701:TYR:O	1:D:705:ASN:HB3	2.15	0.46
2:E:543:LEU:HG	2:E:547:PHE:CE2	2.51	0.46
2:F:409:LEU:HA	2:F:412:VAL:HG12	1.98	0.46
2:E:591:ARG:HG2	2:F:618:HIS:CD2	2.51	0.46
2:I:603:SER:OG	2:I:604:GLY:N	2.48	0.46
1:J:526:ILE:HG12	1:J:790:ASN:ND2	2.31	0.46
2:C:413:ILE:O	2:C:416:ILE:HG13	2.16	0.46
1:D:634:GLU:O	1:D:637:THR:HG22	2.16	0.46
2:I:401:TYR:HD1	2:I:404:ILE:HD12	1.81	0.46
2:K:330:ILE:HG22	2:K:331:ASP:O	2.16	0.46
2:K:384:LEU:HD13	2:K:432:VAL:HG13	1.96	0.46
2:K:429:TRP:CD1	2:K:429:TRP:N	2.82	0.46
1:A:1085:LEU:O	1:A:1089:ALA:N	2.49	0.46
1:A:634:GLU:O	1:A:637:THR:HG22	2.16	0.46
2:B:406:LEU:HD13	2:B:483:LEU:HD13	1.97	0.46
1:D:913:PHE:CZ	1:D:1020:ASP:HA	2.50	0.46
2:E:359:ASP:O	2:E:374:VAL:HG12	2.15	0.46
2:F:233:LEU:HD12	1:D:376:LYS:HA	1.97	0.46
2:F:621:ASP:OD1	2:F:622:SER:N	2.48	0.46
1:G:920:LEU:HD13	1:G:933:ARG:HD3	1.98	0.46
2:B:592:ILE:HA	2:B:595:ARG:HG3	1.98	0.45
1:D:630:LEU:HD23	1:D:630:LEU:HA	1.73	0.45
2:E:429:TRP:HD1	2:E:430:ARG:N	2.14	0.45
2:H:278:PRO:HG2	2:H:296:PRO:HD3	1.98	0.45
1:G:386:PHE:HD2	2:I:631:THR:HG22	1.81	0.45
2:I:644:ILE:O	2:I:663:TYR:HB2	2.16	0.45
1:J:1053:ALA:O	1:J:1057:LEU:N	2.49	0.45
2:L:614:ASP:OD2	2:K:595:ARG:NH2	2.49	0.45
2:L:635:ARG:HH22	1:J:388:SER:HB3	1.81	0.45
1:A:575:LYS:O	1:A:578:THR:HG22	2.17	0.45
2:B:570:SER:HA	2:B:573:LEU:HD23	1.97	0.45
2:C:389:PHE:CE1	2:C:499:PRO:HB3	2.51	0.45
1:D:558:GLU:O	1:D:561:HIS:ND1	2.49	0.45
2:E:290:ASP:OD1	2:E:316:ASN:HB3	2.16	0.45
2:F:333:SER:OG	2:F:334:MET:N	2.49	0.45
1:J:1020:ASP:O	1:J:1024:ILE:HG13	2.17	0.45
2:K:278:PRO:HG3	2:K:294:LEU:O	2.16	0.45
1:D:873:ASP:O	1:D:877:ARG:HG2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:266:LEU:HD23	2:I:570:SER:HB3	1.97	0.45
2:H:543:LEU:HG	2:H:547:PHE:CE2	2.51	0.45
2:I:504:LEU:HA	2:I:507:ILE:HG12	1.98	0.45
2:I:606:LYS:O	2:I:609:ILE:HG13	2.16	0.45
1:J:575:LYS:O	1:J:578:THR:HG22	2.17	0.45
2:L:561:TYR:HE1	2:L:564:TYR:HD2	1.65	0.45
2:L:621:ASP:O	2:L:624:GLY:HA2	2.17	0.45
2:E:581:LEU:HD23	2:E:637:LEU:HB3	1.98	0.45
2:F:357:PHE:HZ	2:F:360:ILE:HB	1.81	0.45
2:F:574:GLU:HG2	2:F:578:LEU:HD13	1.97	0.45
1:G:761:TYR:HE1	1:G:786:LYS:HZ2	1.63	0.45
2:I:578:LEU:O	2:I:582:VAL:HG23	2.17	0.45
1:D:656:THR:HG22	1:D:724:GLN:HG2	1.98	0.45
2:F:292:PHE:HE2	2:F:316:ASN:HA	1.81	0.45
1:G:555:ASP:OD1	1:G:559:ARG:NH1	2.50	0.45
1:G:641:ASN:O	1:G:642:ILE:HG13	2.16	0.45
1:J:537:LEU:HD21	1:J:552:TYR:CE1	2.51	0.45
2:L:347:SER:O	2:L:356:LYS:NZ	2.48	0.45
2:F:654:ASP:OD2	1:D:420:LYS:HG3	2.17	0.45
1:D:641:ASN:O	1:D:642:ILE:HG13	2.16	0.45
1:D:696:LEU:HB2	1:D:697:PRO:HD3	1.99	0.45
2:L:261:ASN:OD1	2:L:262:ILE:N	2.49	0.45
2:B:640:LEU:HD21	1:A:378:LEU:HD13	1.98	0.45
1:D:538:LYS:HG3	1:D:539:ASP:OD1	2.17	0.45
1:D:555:ASP:OD1	1:D:559:ARG:NH1	2.50	0.45
1:D:509:PRO:HD3	1:D:827:TYR:HD2	1.82	0.45
1:G:552:TYR:OH	1:G:1000:ARG:HD2	2.16	0.45
1:G:539:ASP:HB2	1:G:541:ASN:HD21	1.81	0.45
1:G:946:ARG:HD2	1:G:955:VAL:HG23	1.98	0.45
2:H:354:LEU:HD13	2:H:416:ILE:HD11	1.98	0.45
1:J:445:TYR:OH	1:J:447:CYS:HB3	2.17	0.45
2:L:654:ASP:OD1	2:L:655:GLU:N	2.50	0.45
1:A:476:PRO:HB2	1:A:479:TYR:HD1	1.80	0.45
2:C:357:PHE:CZ	2:C:360:ILE:HB	2.52	0.45
2:H:338:LYS:O	2:H:342:ILE:HG12	2.17	0.45
2:K:403:TRP:CE3	2:K:550:LYS:HG3	2.51	0.45
2:K:578:LEU:O	2:K:582:VAL:HG22	2.17	0.45
2:B:389:PHE:CG	2:B:499:PRO:HG3	2.51	0.45
2:C:618:HIS:CG	2:B:591:ARG:HD2	2.52	0.45
2:C:630:LEU:HB2	1:A:386:PHE:CE2	2.52	0.45
2:F:346:TRP:CZ2	2:F:448:PHE:HB3	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:360:ASP:OD1	1:G:363:TYR:N	2.50	0.45
1:G:610:SER:N	1:G:613:SER:HG	2.15	0.45
1:J:452:ARG:O	1:J:454:GLN:HG3	2.17	0.45
1:J:960:ASP:HB3	1:J:992:LEU:HD11	1.99	0.45
1:D:550:LEU:HD13	1:D:630:LEU:HD11	1.99	0.45
2:E:619:GLN:O	2:E:626:PRO:HA	2.17	0.45
2:K:371:ILE:HG13	2:K:371:ILE:O	2.15	0.45
2:K:401:TYR:HD1	2:K:404:ILE:HD12	1.81	0.45
2:L:356:LYS:HB3	2:L:376:ASP:OD1	2.17	0.45
2:B:639:LYS:HB3	2:B:663:TYR:CD2	2.51	0.44
2:C:330:ILE:HG13	2:C:330:ILE:O	2.17	0.44
1:G:429:LEU:HB3	2:I:657:ASN:ND2	2.29	0.44
2:L:327:LEU:O	2:L:330:ILE:HD11	2.17	0.44
2:C:507:ILE:HG21	2:C:530:ILE:HG21	1.99	0.44
1:D:392:ILE:HA	1:D:393:PRO:HD3	1.85	0.44
2:F:398:THR:HG23	2:F:401:TYR:H	1.81	0.44
2:F:621:ASP:O	2:F:624:GLY:HA2	2.17	0.44
2:I:621:ASP:OD1	2:I:622:SER:N	2.49	0.44
2:K:327:LEU:HB2	2:K:371:ILE:O	2.16	0.44
2:K:398:THR:HG23	2:K:401:TYR:H	1.80	0.44
1:A:1055:VAL:HG12	1:A:1056:LEU:HD12	2.00	0.44
1:A:896:THR:HG22	1:A:899:GLU:HG2	1.99	0.44
1:A:510:ASP:OD1	1:A:936:ARG:NH1	2.51	0.44
2:F:323:VAL:HG23	2:F:377:TYR:HA	1.99	0.44
1:G:447:CYS:SG	1:G:450:ASP:HB2	2.57	0.44
1:J:526:ILE:HG12	1:J:790:ASN:HD22	1.82	0.44
2:C:355:ILE:HD11	2:C:376:ASP:O	2.18	0.44
2:C:401:TYR:HA	2:C:404:ILE:HD12	1.99	0.44
1:D:1015:HIS:ND1	1:D:1036:THR:OG1	2.29	0.44
2:E:294:LEU:HB3	2:E:311:PHE:CE1	2.52	0.44
2:E:635:ARG:NH1	1:D:351:THR:OG1	2.48	0.44
1:G:902:LYS:H	1:G:905:THR:HG1	1.60	0.44
2:H:351:CYS:HB3	2:H:354:LEU:HB3	2.00	0.44
2:H:621:ASP:N	2:H:625:LYS:O	2.32	0.44
2:I:295:VAL:HG11	2:I:312:LYS:HE3	1.98	0.44
1:J:546:LEU:HD12	1:J:629:GLN:HG2	1.99	0.44
1:J:891:GLU:OE1	1:J:990:LYS:NZ	2.41	0.44
1:J:963:VAL:HG13	1:J:964:ASN:N	2.32	0.44
1:A:650:LEU:HG	1:A:670:LEU:O	2.17	0.44
1:D:919:GLU:HA	1:D:933:ARG:O	2.17	0.44
1:G:761:TYR:HE1	1:G:786:LYS:HG3	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:548:TYR:OH	2:I:541:HIS:O	2.34	0.44
2:H:563:GLU:OE2	2:I:442:LYS:NZ	2.39	0.44
2:I:395:PHE:HA	2:I:396:PRO:HD3	1.73	0.44
2:L:450:ASP:OD1	2:L:451:LEU:N	2.50	0.44
2:B:527:LYS:HA	2:B:530:ILE:HG22	1.99	0.44
2:C:610:ILE:HG13	2:C:611:LEU:N	2.33	0.44
2:E:615:TYR:OH	1:D:345:ASP:OD2	2.34	0.44
1:G:537:LEU:O	1:G:1000:ARG:NH2	2.50	0.44
1:G:423:THR:HB	1:G:427:PRO:HG3	1.98	0.44
1:G:864:SER:O	1:G:867:THR:HG22	2.17	0.44
2:H:460:VAL:O	1:J:1029:PRO:HB3	2.18	0.44
2:C:630:LEU:O	2:C:634:LEU:HD12	2.18	0.44
2:C:657:ASN:ND2	1:A:415:SER:HB2	2.33	0.44
1:D:347:PHE:CD1	1:D:347:PHE:N	2.84	0.44
2:F:620:VAL:O	1:D:441:ALA:HA	2.17	0.44
1:D:597:GLU:HG3	1:D:598:SER:N	2.32	0.44
2:F:612:PHE:O	2:F:616:VAL:HG12	2.18	0.44
1:G:634:GLU:O	1:G:637:THR:HG22	2.18	0.44
1:G:351:THR:HG21	2:H:635:ARG:CZ	2.47	0.44
2:I:287:ILE:O	2:I:365:LYS:HE3	2.18	0.44
1:J:1056:LEU:HD23	1:J:1081:LYS:HG3	1.99	0.44
2:L:552:PHE:O	2:L:556:GLU:HG2	2.18	0.44
2:B:641:ASP:OD1	1:A:378:LEU:N	2.51	0.44
2:B:427:LEU:O	2:B:482:LEU:HD22	2.18	0.44
2:C:652:THR:OG1	2:C:657:ASN:HB2	2.18	0.44
1:D:913:PHE:HZ	1:D:1020:ASP:HA	1.83	0.44
2:E:362:GLN:HG3	2:E:371:ILE:HG22	1.99	0.44
2:F:426:THR:HG21	2:F:445:HIS:ND1	2.32	0.44
1:J:371:PRO:HG2	1:J:372:TYR:H	1.82	0.44
1:J:550:LEU:HD21	1:J:554:PHE:CE2	2.52	0.44
1:J:877:ARG:HH12	1:J:879:TYR:HD2	1.66	0.44
1:A:540:GLU:OE2	1:A:871:ASN:ND2	2.51	0.44
1:A:966:ASN:O	1:A:967:HIS:HB2	2.17	0.44
1:D:1030:ARG:CB	2:B:457:THR:H	2.30	0.44
2:C:626:PRO:HB3	2:B:591:ARG:HH22	1.83	0.44
2:B:577:ARG:NH2	2:B:638:ASN:OD1	2.45	0.44
2:H:353:ASN:O	2:H:442:LYS:HA	2.18	0.44
2:H:621:ASP:O	2:H:624:GLY:N	2.49	0.44
1:J:650:LEU:HG	1:J:670:LEU:O	2.18	0.44
1:J:880:PHE:CE1	1:J:990:LYS:HB3	2.52	0.44
2:K:248:PRO:HD2	2:K:251:ARG:HG3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:626:PRO:HG2	2:K:677:ILE:O	2.18	0.44
1:A:627:LEU:HD22	1:A:648:PHE:HD2	1.83	0.43
2:C:261:ASN:OD1	2:C:262:ILE:N	2.51	0.43
2:C:487:SER:O	2:C:490:ILE:HG22	2.18	0.43
1:G:754:ASN:ND2	1:G:754:ASN:O	2.51	0.43
1:G:509:PRO:HD3	1:G:827:TYR:HD1	1.83	0.43
2:K:353:ASN:O	2:K:442:LYS:HA	2.18	0.43
2:L:589:PHE:O	2:K:618:HIS:NE2	2.49	0.43
2:L:618:HIS:HD2	2:K:591:ARG:HA	1.83	0.43
1:A:1015:HIS:HD1	1:A:1036:THR:HG1	1.63	0.43
1:A:893:LYS:O	1:A:957:PHE:HA	2.18	0.43
2:B:385:TYR:HB2	2:B:429:TRP:HD1	1.80	0.43
1:D:1029:PRO:HG2	1:D:1032:GLN:OE1	2.19	0.43
1:D:482:LEU:HD21	1:D:828:LEU:HB2	2.00	0.43
2:E:627:ILE:HD11	1:D:343:TYR:CD2	2.52	0.43
2:F:409:LEU:CD1	2:F:441:ILE:HG21	2.48	0.43
2:I:423:ILE:CG2	2:I:475:ASP:HB3	2.48	0.43
1:J:542:PHE:CE2	1:J:997:VAL:HG12	2.53	0.43
2:K:388:HIS:ND1	2:K:397:ILE:HG13	2.33	0.43
1:A:789:LEU:HA	1:A:852:TYR:CD1	2.53	0.43
1:D:872:TYR:HA	1:D:1004:LEU:HD13	1.99	0.43
2:E:595:ARG:NH2	2:F:614:ASP:OD2	2.51	0.43
1:G:994:ARG:O	1:G:996:ASN:N	2.52	0.43
1:J:418:ASN:C	1:J:420:LYS:H	2.20	0.43
1:A:416:SER:HB2	1:A:710:ASN:CB	2.48	0.43
2:C:638:ASN:CG	2:B:274:LEU:HD11	2.38	0.43
1:D:759:GLU:OE1	2:C:516:ARG:NH1	2.52	0.43
1:D:760:PHE:CE1	1:D:771:LEU:HD23	2.53	0.43
2:E:326:ARG:CZ	2:E:328:PRO:HB3	2.48	0.43
2:F:611:LEU:HA	2:F:611:LEU:HD12	1.87	0.43
2:I:308:THR:HG22	2:I:310:LEU:H	1.84	0.43
2:I:399:ASN:OD1	2:I:400:ASN:N	2.52	0.43
1:J:598:SER:HA	1:J:601:ILE:HG22	2.00	0.43
1:A:523:TYR:CE2	1:A:627:LEU:HD21	2.52	0.43
2:C:291:TYR:HD1	2:C:315:SER:HA	1.83	0.43
2:C:407:VAL:HG21	2:C:554:VAL:HG21	2.01	0.43
1:D:360:ASP:OD1	1:D:363:TYR:N	2.47	0.43
1:D:513:ASN:HB3	1:D:515:TYR:CE2	2.54	0.43
2:F:301:ASN:ND2	2:F:308:THR:HA	2.34	0.43
2:F:352:THR:OG1	2:F:353:ASN:N	2.51	0.43
2:F:405:TYR:CD1	2:F:441:ILE:HD11	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:483:LEU:HD23	2:L:522:PHE:HE1	1.83	0.43
1:A:447:CYS:SG	1:A:450:ASP:HB2	2.59	0.43
2:C:401:TYR:HD1	2:C:404:ILE:HD12	1.84	0.43
2:C:427:LEU:HD23	2:C:427:LEU:O	2.18	0.43
1:D:999:TYR:OH	1:D:1026:ILE:HD13	2.19	0.43
2:F:254:ASP:OD1	2:F:254:ASP:N	2.51	0.43
2:I:423:ILE:HG21	2:I:475:ASP:CB	2.48	0.43
2:I:406:LEU:HD11	2:I:525:VAL:HG11	2.01	0.43
1:A:815:LYS:HD3	1:A:815:LYS:HA	1.83	0.43
2:C:353:ASN:HA	2:C:442:LYS:HG2	2.01	0.43
2:C:652:THR:CG2	2:C:653:PRO:HD2	2.49	0.43
2:E:357:PHE:HD1	2:E:375:PHE:HE1	1.66	0.43
2:E:408:GLN:O	2:E:411:ASN:HB3	2.19	0.43
2:F:349:ILE:HG22	2:F:419:GLN:NE2	2.34	0.43
2:H:577:ARG:HA	2:H:580:ARG:HE	1.83	0.43
2:I:468:ILE:O	2:I:472:GLN:HG3	2.19	0.43
1:J:694:ASN:O	1:J:697:PRO:HD2	2.19	0.43
2:L:397:ILE:HD11	2:L:486:LEU:HB3	2.01	0.43
2:B:405:TYR:HA	2:B:441:ILE:HD13	1.99	0.43
2:E:330:ILE:HG22	2:E:369:LEU:HB3	1.99	0.43
1:G:529:MET:O	1:G:533:VAL:HG23	2.19	0.43
1:G:818:CYS:SG	1:G:819:PHE:N	2.92	0.43
1:A:445:TYR:OH	1:A:447:CYS:HB3	2.19	0.43
2:C:288:VAL:O	2:C:291:TYR:N	2.32	0.43
1:D:345:ASP:O	1:D:349:ASP:HB2	2.19	0.43
2:E:294:LEU:HD23	2:E:311:PHE:CE1	2.54	0.43
2:E:327:LEU:HB2	2:E:371:ILE:O	2.18	0.43
2:E:591:ARG:HG2	2:F:618:HIS:HD2	1.83	0.43
2:E:612:PHE:CE2	2:E:640:LEU:HD22	2.53	0.43
2:F:419:GLN:OE1	2:F:419:GLN:N	2.52	0.43
1:G:523:TYR:OH	1:G:623:ASN:OD1	2.29	0.43
1:J:695:ILE:O	1:J:698:TYR:HB2	2.19	0.43
2:K:427:LEU:HA	2:K:427:LEU:HD23	1.83	0.43
2:L:648:LEU:HG	2:L:663:TYR:HE1	1.84	0.43
1:A:853:CYS:HB3	1:A:858:LEU:HD12	2.01	0.43
1:D:526:ILE:HD11	1:D:851:ILE:HG21	2.01	0.43
2:E:296:PRO:HA	2:E:311:PHE:CB	2.48	0.43
2:E:324:LEU:HD22	2:E:373:LEU:O	2.19	0.43
2:E:354:LEU:HD13	2:E:416:ILE:HD11	2.01	0.43
2:E:652:THR:HB	2:E:654:ASP:H	1.84	0.43
1:G:659:SER:C	1:G:661:ASP:H	2.22	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:382:LEU:O	2:H:434:ILE:HG22	2.19	0.43
2:I:260:ASN:O	2:I:263:ARG:NH1	2.52	0.43
2:I:355:ILE:HG12	2:I:443:LEU:O	2.19	0.43
2:L:250:GLU:OE2	1:J:387:LYS:NZ	2.49	0.43
1:A:1020:ASP:O	1:A:1024:ILE:HG13	2.19	0.42
1:A:961:TYR:CD2	1:A:989:THR:HG21	2.54	0.42
2:E:654:ASP:O	2:E:656:LEU:N	2.51	0.42
2:F:504:LEU:HA	2:F:507:ILE:HG12	2.01	0.42
2:F:588:ILE:HG21	2:F:609:ILE:HD11	2.01	0.42
2:H:635:ARG:HG2	2:H:639:LYS:HE2	2.00	0.42
2:I:435:THR:O	2:I:440:ARG:HB2	2.19	0.42
1:J:675:ILE:O	1:J:675:ILE:HG13	2.18	0.42
2:K:346:TRP:CZ2	2:K:421:LEU:HD13	2.54	0.42
1:A:539:ASP:O	1:A:1000:ARG:NH1	2.53	0.42
1:A:946:ARG:NH1	1:A:955:VAL:HG13	2.34	0.42
1:D:529:MET:O	1:D:533:VAL:HG23	2.19	0.42
2:H:671:GLU:OE2	2:H:675:ARG:NH2	2.50	0.42
2:I:408:GLN:NE2	2:I:441:ILE:H	2.16	0.42
2:L:338:LYS:O	2:L:342:ILE:HG12	2.18	0.42
2:L:421:LEU:HB3	2:L:448:PHE:HZ	1.84	0.42
2:B:253:ALA:C	2:B:255:GLN:H	2.23	0.42
2:B:640:LEU:HD11	2:B:670:ILE:HD12	2.01	0.42
2:C:584:LYS:HE2	2:C:674:PHE:CE2	2.55	0.42
2:C:581:LEU:HD21	2:C:640:LEU:HD22	2.01	0.42
2:E:270:ASN:OD1	2:E:271:LEU:N	2.52	0.42
2:E:629:ASP:O	2:E:633:VAL:HG23	2.19	0.42
1:G:343:TYR:HA	1:G:344:PRO:HA	1.85	0.42
1:G:992:LEU:O	1:G:992:LEU:HD12	2.18	0.42
2:K:389:PHE:CE2	2:K:429:TRP:HZ3	2.34	0.42
2:C:257:PHE:CZ	2:B:579:PHE:HD2	2.37	0.42
2:B:591:ARG:O	2:B:595:ARG:HG3	2.19	0.42
2:C:391:ASN:CG	2:C:392:PHE:H	2.23	0.42
2:C:592:ILE:CD1	2:B:653:PRO:HG3	2.49	0.42
2:C:590:GLY:O	2:C:595:ARG:NH1	2.52	0.42
1:D:1019:ASN:O	1:D:1023:HIS:ND1	2.53	0.42
1:D:641:ASN:C	1:D:642:ILE:HG13	2.40	0.42
1:D:798:ASP:OD1	1:D:802:GLU:N	2.52	0.42
2:E:265:ASP:O	2:E:268:LYS:HB3	2.20	0.42
2:E:549:ASP:O	2:E:552:PHE:HB2	2.20	0.42
2:F:401:TYR:HA	2:F:404:ILE:HD12	2.01	0.42
1:G:641:ASN:C	1:G:642:ILE:HG13	2.39	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:944:ILE:O	1:G:957:PHE:N	2.52	0.42
2:I:620:VAL:HG12	2:I:621:ASP:O	2.20	0.42
1:J:471:ASN:OD1	1:J:473:TYR:N	2.50	0.42
2:K:426:THR:OG1	2:K:447:ASN:N	2.52	0.42
2:L:476:TYR:O	2:L:529:LEU:HD23	2.20	0.42
2:L:619:GLN:HE22	2:L:632:HIS:HB3	1.84	0.42
1:A:464:ILE:HA	1:A:477:PRO:HB2	2.02	0.42
1:G:470:ILE:HD12	1:G:470:ILE:H	1.84	0.42
2:I:280:SER:HB2	2:I:283:VAL:CG1	2.46	0.42
1:J:537:LEU:HD23	1:J:537:LEU:O	2.20	0.42
1:J:791:GLY:O	1:J:851:ILE:HG13	2.19	0.42
1:J:992:LEU:O	1:J:992:LEU:HD12	2.20	0.42
1:J:994:ARG:HG3	1:J:995:ARG:N	2.35	0.42
1:J:997:VAL:HG23	1:J:998:VAL:N	2.35	0.42
2:L:601:SER:HB2	2:L:610:ILE:HD12	2.02	0.42
1:J:746:PHE:O	1:J:749:ILE:HG13	2.20	0.42
2:L:578:LEU:O	2:L:582:VAL:HG23	2.20	0.42
2:L:652:THR:CG2	2:L:653:PRO:HD2	2.49	0.42
1:A:534:VAL:HG12	1:A:865:VAL:HB	2.00	0.42
2:B:484:PHE:CD1	2:B:488:ILE:HD13	2.55	0.42
1:D:962:VAL:HG21	1:D:994:ARG:HB3	2.01	0.42
2:E:426:THR:OG1	2:E:447:ASN:HB2	2.19	0.42
2:E:633:VAL:HG11	2:F:583:ASN:HD21	1.85	0.42
2:F:242:LEU:O	2:F:246:LEU:HG	2.20	0.42
2:F:386:ASP:O	2:F:390:VAL:HB	2.20	0.42
2:F:487:SER:O	2:F:490:ILE:HG22	2.19	0.42
2:F:484:PHE:CD2	2:F:507:ILE:HD12	2.55	0.42
1:G:959:ASP:OD2	1:G:1069:ILE:HD11	2.20	0.42
2:H:388:HIS:CE1	2:H:405:TYR:HH	2.36	0.42
2:H:586:ASN:OD1	2:I:613:TYR:OH	2.10	0.42
2:K:577:ARG:HH12	1:J:370:MET:CG	2.28	0.42
2:K:591:ARG:HB2	2:K:594:SER:CB	2.50	0.42
2:L:250:GLU:O	2:L:251:ARG:HD3	2.19	0.42
1:D:645:ASN:O	1:D:649:GLY:HA3	2.20	0.42
2:F:521:LYS:O	2:F:525:VAL:HG23	2.19	0.42
1:G:475:VAL:HA	1:G:476:PRO:HD3	1.89	0.42
2:I:345:ILE:HG13	2:I:346:TRP:N	2.34	0.42
2:I:589:PHE:CD1	2:I:610:ILE:HG23	2.55	0.42
1:J:634:GLU:O	1:J:637:THR:HG22	2.20	0.42
2:K:589:PHE:CG	2:K:613:TYR:CD2	3.08	0.42
2:L:577:ARG:NE	2:L:641:ASP:OD2	2.45	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:750:ARG:NH1	1:A:843:PRO:O	2.53	0.42
2:E:294:LEU:HD12	2:E:294:LEU:H	1.84	0.42
2:F:610:ILE:O	2:F:613:TYR:HB3	2.20	0.42
2:I:629:ASP:OD1	2:I:630:LEU:N	2.53	0.42
2:L:327:LEU:HB2	2:L:371:ILE:HG23	2.01	0.42
1:A:471:ASN:OD1	1:A:473:TYR:N	2.49	0.42
2:B:426:THR:OG1	2:B:447:ASN:N	2.52	0.42
1:D:639:ASN:HB3	1:D:641:ASN:ND2	2.35	0.42
2:E:578:LEU:O	2:E:582:VAL:HG22	2.20	0.42
2:F:404:ILE:HG12	2:F:554:VAL:HG22	2.02	0.42
1:G:440:ASN:CG	2:I:615:TYR:HA	2.40	0.42
2:I:473:GLN:HE22	2:I:533:ASN:CG	2.18	0.42
1:J:813:ASN:HA	1:J:814:PRO:HD3	1.86	0.42
1:J:509:PRO:HD3	1:J:827:TYR:HD1	1.84	0.42
2:K:502:TYR:CD1	2:K:506:GLU:OE1	2.73	0.42
2:L:652:THR:HB	2:L:654:ASP:OD1	2.19	0.42
1:A:756:LEU:HD21	1:A:789:LEU:HD22	2.02	0.41
2:B:324:LEU:HD11	2:B:361:PHE:HZ	1.84	0.41
2:E:407:VAL:HG11	2:E:554:VAL:HG11	2.02	0.41
1:G:448:LEU:O	1:G:452:ARG:HG2	2.20	0.41
1:G:637:THR:HG23	1:G:640:HIS:H	1.85	0.41
2:I:263:ARG:NH1	2:I:263:ARG:HB3	2.35	0.41
2:K:401:TYR:HA	2:K:404:ILE:HD12	2.02	0.41
2:L:261:ASN:OD1	2:L:262:ILE:HG12	2.20	0.41
1:A:509:PRO:HD3	1:A:827:TYR:HD2	1.84	0.41
1:D:924:ASP:OD1	1:D:924:ASP:N	2.50	0.41
2:F:597:ASP:OD1	2:F:598:ILE:N	2.52	0.41
2:H:629:ASP:O	2:H:633:VAL:HG23	2.20	0.41
1:J:864:SER:O	1:J:867:THR:HG22	2.21	0.41
1:J:876:PHE:CD1	1:J:895:LEU:HB2	2.56	0.41
2:K:273:ILE:HG13	2:K:274:LEU:N	2.34	0.41
1:D:920:LEU:HA	1:D:920:LEU:HD13	1.92	0.41
2:F:429:TRP:HE1	2:F:485:ASN:HB2	1.85	0.41
2:L:324:LEU:HD21	2:L:372:CYS:HB3	2.02	0.41
2:C:392:PHE:HB3	2:C:393:PRO:HD3	2.01	0.41
2:F:475:ASP:OD1	2:F:476:TYR:N	2.54	0.41
2:F:519:ASP:O	2:F:522:PHE:N	2.54	0.41
2:I:291:TYR:HD1	2:I:315:SER:HA	1.84	0.41
2:I:484:PHE:CD2	2:I:507:ILE:HD12	2.56	0.41
1:J:553:LEU:O	1:J:557:MET:HG3	2.19	0.41
2:K:368:ASP:OD1	2:K:370:SER:OG	2.38	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:543:LEU:HG	2:K:547:PHE:CE2	2.55	0.41
2:L:586:ASN:HB3	2:K:617:PHE:CD2	2.56	0.41
2:L:597:ASP:HB3	2:L:599:ASN:O	2.20	0.41
2:C:291:TYR:CE2	2:C:374:VAL:HG21	2.55	0.41
2:F:619:GLN:OE1	2:F:632:HIS:ND1	2.53	0.41
2:F:630:LEU:O	2:F:634:LEU:HD12	2.21	0.41
1:G:810:LYS:HE3	1:G:821:TRP:CZ2	2.55	0.41
2:H:294:LEU:HD23	2:H:311:PHE:CD2	2.55	0.41
2:H:406:LEU:HG	2:H:547:PHE:CZ	2.56	0.41
2:L:330:ILE:HG22	2:L:332:LYS:H	1.85	0.41
1:A:739:LEU:HD12	1:A:847:PRO:HB2	2.01	0.41
1:D:454:GLN:HE22	1:A:458:GLY:HA3	1.86	0.41
1:D:476:PRO:HA	1:D:477:PRO:HD3	1.94	0.41
1:D:764:ILE:H	1:D:764:ILE:HG13	1.73	0.41
2:H:473:GLN:O	2:H:476:TYR:HB2	2.21	0.41
2:H:589:PHE:CD1	2:H:613:TYR:HD2	2.39	0.41
1:J:370:MET:HE3	1:J:370:MET:HB3	1.90	0.41
2:H:460:VAL:HG22	1:J:560:SER:HA	2.02	0.41
1:J:564:ILE:H	1:J:564:ILE:HD12	1.85	0.41
2:L:416:ILE:HG22	2:L:421:LEU:O	2.21	0.41
2:L:469:GLU:O	2:L:473:GLN:HG2	2.21	0.41
1:A:553:LEU:O	1:A:557:MET:HG3	2.20	0.41
2:B:403:TRP:O	2:B:407:VAL:HG23	2.21	0.41
2:E:652:THR:N	2:E:653:PRO:HA	2.36	0.41
2:F:550:LYS:O	2:F:553:MET:HB3	2.20	0.41
2:H:578:LEU:O	2:H:582:VAL:HG22	2.20	0.41
2:H:630:LEU:O	2:H:634:LEU:HD12	2.20	0.41
2:I:521:LYS:HD3	2:I:547:PHE:HB3	2.03	0.41
1:A:650:LEU:HD13	1:A:728:VAL:HG11	2.01	0.41
1:A:444:ASP:HB3	1:A:801:ASN:ND2	2.36	0.41
2:B:468:ILE:O	2:B:472:GLN:HG3	2.21	0.41
2:C:352:THR:O	2:C:353:ASN:HB2	2.21	0.41
1:G:509:PRO:HD3	1:G:827:TYR:CD1	2.55	0.41
1:G:517:ASN:O	1:G:520:ILE:HG13	2.21	0.41
1:G:894:LEU:H	1:G:894:LEU:HD12	1.86	0.41
1:J:1035:ASP:OD1	1:J:1037:ALA:N	2.53	0.41
1:A:550:LEU:HB2	1:A:570:PHE:HE2	1.85	0.41
2:B:549:ASP:O	2:B:552:PHE:HB2	2.21	0.41
2:B:629:ASP:O	2:B:633:VAL:HG23	2.21	0.41
2:E:288:VAL:HG11	2:E:366:PHE:CE1	2.56	0.41
1:G:634:GLU:CD	1:G:642:ILE:HA	2.41	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:423:ILE:N	2:H:475:ASP:OD2	2.46	0.41
2:I:654:ASP:OD1	2:I:655:GLU:N	2.53	0.41
2:L:395:PHE:HA	2:L:396:PRO:HD3	1.75	0.41
1:A:946:ARG:HG3	1:A:957:PHE:HD1	1.86	0.41
2:C:406:LEU:HD12	2:C:522:PHE:CE1	2.56	0.41
2:F:397:ILE:HG23	2:F:397:ILE:O	2.21	0.41
1:G:813:ASN:HA	1:G:814:PRO:HD3	1.92	0.41
1:J:641:ASN:C	1:J:642:ILE:HG13	2.41	0.41
2:L:552:PHE:HE1	2:K:544:THR:HG21	1.84	0.41
2:B:652:THR:OG1	2:B:654:ASP:N	2.54	0.41
2:C:628:MET:HE3	2:C:628:MET:HB2	1.96	0.41
2:C:640:LEU:HD11	2:C:670:ILE:HD12	2.03	0.41
1:D:741:LEU:HB2	1:D:746:PHE:CE2	2.55	0.41
1:D:863:PHE:HD1	1:D:867:THR:HG21	1.86	0.41
2:E:416:ILE:HG22	2:E:421:LEU:O	2.20	0.41
1:G:994:ARG:O	1:G:997:VAL:HG22	2.20	0.41
2:I:589:PHE:CG	2:I:590:GLY:N	2.89	0.41
1:J:471:ASN:HB3	1:J:474:GLU:HB3	2.03	0.41
1:J:963:VAL:CG1	1:J:993:VAL:HA	2.50	0.41
2:F:508:THR:HA	2:F:509:PRO:HD3	1.96	0.40
2:F:584:LYS:O	2:F:587:CYS:HB3	2.21	0.40
1:G:913:PHE:HZ	1:G:1020:ASP:HA	1.86	0.40
1:J:979:LEU:H	1:J:979:LEU:HD12	1.86	0.40
2:K:291:TYR:HB3	2:K:313:VAL:CG2	2.46	0.40
2:C:654:ASP:C	2:C:656:LEU:H	2.23	0.40
2:F:548:TYR:HD1	2:F:548:TYR:HA	1.71	0.40
1:G:913:PHE:CZ	1:G:1020:ASP:HA	2.56	0.40
1:G:575:LYS:O	1:G:578:THR:HG22	2.21	0.40
1:G:739:LEU:HD12	1:G:847:PRO:HB2	2.02	0.40
2:H:405:TYR:HD1	2:H:441:ILE:CD1	2.34	0.40
2:I:352:THR:C	2:I:354:LEU:H	2.24	0.40
1:J:641:ASN:O	1:J:642:ILE:HG13	2.20	0.40
2:L:589:PHE:CD1	2:L:610:ILE:HG23	2.57	0.40
1:A:732:PRO:O	1:A:787:TYR:OH	2.18	0.40
2:C:434:ILE:HG13	2:C:440:ARG:O	2.22	0.40
2:C:487:SER:OG	2:C:515:MET:SD	2.71	0.40
1:D:539:ASP:O	1:D:1000:ARG:NH1	2.52	0.40
2:E:353:ASN:O	2:E:442:LYS:HA	2.21	0.40
2:F:291:TYR:HB3	2:F:313:VAL:HG13	2.03	0.40
2:I:291:TYR:CE2	2:I:374:VAL:HG21	2.56	0.40
2:I:678:THR:O	2:I:679:GLN:HB2	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:526:ILE:HA	1:J:527:PRO:HD3	1.95	0.40
1:J:778:LEU:HD22	1:J:784:ILE:HD11	2.04	0.40
1:J:839:LYS:HD3	1:J:842:TYR:CE2	2.56	0.40
1:J:961:TYR:CE2	1:J:989:THR:HG21	2.55	0.40
2:K:339:ILE:HG23	2:K:360:ILE:HD13	2.02	0.40
1:A:641:ASN:C	1:A:642:ILE:HG13	2.42	0.40
2:B:584:LYS:HD2	1:A:378:LEU:HD21	2.02	0.40
2:C:231:TYR:O	2:C:233:LEU:HG	2.22	0.40
2:C:353:ASN:H	2:C:442:LYS:HZ2	1.69	0.40
1:D:634:GLU:OE2	1:D:644:LEU:HB2	2.21	0.40
2:E:335:ASN:HA	2:E:336:PRO:HD2	1.90	0.40
1:G:507:LEU:HD12	1:G:517:ASN:HB3	2.03	0.40
1:G:620:GLN:HE22	1:G:848:GLU:C	2.23	0.40
1:G:739:LEU:CD1	1:G:847:PRO:HB2	2.52	0.40
2:I:352:THR:O	2:I:353:ASN:HB2	2.21	0.40
2:I:387:TYR:CE2	2:I:434:ILE:HD13	2.57	0.40
1:J:1002:VAL:HA	1:J:1005:LEU:HD12	2.04	0.40
1:J:824:PHE:CD2	1:J:829:VAL:HG22	2.56	0.40
2:L:429:TRP:HE1	2:L:485:ASN:CB	2.34	0.40
2:C:653:PRO:HB3	2:B:592:ILE:HD12	2.04	0.40
2:C:233:LEU:O	1:A:377:LEU:HD13	2.22	0.40
2:F:234:TYR:HA	1:D:377:LEU:HD12	2.03	0.40
1:D:824:PHE:CD2	1:D:829:VAL:HG22	2.56	0.40
2:E:400:ASN:O	2:E:404:ILE:HG12	2.21	0.40
1:G:731:LEU:HA	1:G:732:PRO:HD3	1.84	0.40
2:H:416:ILE:HG21	2:H:423:ILE:HG12	2.03	0.40
2:I:399:ASN:O	2:I:402:LEU:HB2	2.22	0.40
1:J:343:TYR:HA	1:J:344:PRO:HA	1.82	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	687/776 (88%)	652 (95%)	34 (5%)	1 (0%)	53	87
1	D	663/776 (85%)	622 (94%)	39 (6%)	2 (0%)	43	79
1	G	665/776 (86%)	631 (95%)	32 (5%)	2 (0%)	43	79
1	J	661/776 (85%)	624 (94%)	35 (5%)	2 (0%)	43	79
2	B	421/465 (90%)	397 (94%)	24 (6%)	0	100	100
2	C	440/465 (95%)	417 (95%)	23 (5%)	0	100	100
2	E	408/465 (88%)	384 (94%)	24 (6%)	0	100	100
2	F	438/465 (94%)	415 (95%)	22 (5%)	1 (0%)	49	83
2	H	416/465 (90%)	394 (95%)	21 (5%)	1 (0%)	49	83
2	I	429/465 (92%)	404 (94%)	24 (6%)	1 (0%)	49	83
2	K	423/465 (91%)	408 (96%)	15 (4%)	0	100	100
2	L	437/465 (94%)	416 (95%)	21 (5%)	0	100	100
All	All	6088/6824 (89%)	5764 (95%)	314 (5%)	10 (0%)	49	83

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	J	455	ILE
1	G	616	ARG
2	F	397	ILE
1	A	660	CYS
1	G	715	THR
2	H	438	PRO
1	J	371	PRO
2	I	397	ILE
1	D	678	ILE
1	D	344	PRO

5.3.2 Protein sidechains ⓘ

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

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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	509/712 (72%)	496 (97%)	13 (3%)	49	76
1	D	465/712 (65%)	458 (98%)	7 (2%)	67	85
1	G	469/712 (66%)	459 (98%)	10 (2%)	56	80
1	J	462/712 (65%)	454 (98%)	8 (2%)	63	84
2	B	332/444 (75%)	325 (98%)	7 (2%)	56	80
2	C	352/444 (79%)	348 (99%)	4 (1%)	76	88
2	E	297/444 (67%)	294 (99%)	3 (1%)	78	89
2	F	348/444 (78%)	343 (99%)	5 (1%)	69	86
2	H	307/444 (69%)	300 (98%)	7 (2%)	53	78
2	I	331/444 (74%)	329 (99%)	2 (1%)	87	94
2	K	328/444 (74%)	321 (98%)	7 (2%)	56	80
2	L	375/444 (84%)	370 (99%)	5 (1%)	71	87
All	All	4575/6400 (72%)	4497 (98%)	78 (2%)	63	84

All (78) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	438	MET
1	G	513	ASN
1	G	521	GLN
1	G	524	ARG
1	G	617	ASN
1	G	636	GLN
1	G	896	THR
1	G	990	LYS
1	G	998	VAL
1	G	1025	ASN
2	L	295	VAL
2	L	307	LYS
2	L	346	TRP
2	L	434	ILE
2	L	497	THR
2	K	273	ILE
2	K	295	VAL
2	K	429	TRP
2	K	503	ARG

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Mol	Chain	Res	Type
2	K	548	TYR
2	K	641	ASP
2	K	648	LEU
2	E	386	ASP
2	E	504	LEU
2	E	641	ASP
2	F	228	LEU
2	F	295	VAL
2	F	306	ASN
2	F	448	PHE
2	F	619	GLN
1	D	485	THR
1	D	494	PHE
1	D	524	ARG
1	D	640	HIS
1	D	678	ILE
1	D	704	LYS
1	D	991	ARG
2	H	295	VAL
2	H	309	THR
2	H	369	LEU
2	H	386	ASP
2	H	516	ARG
2	H	613	TYR
2	H	658	CYS
2	I	295	VAL
2	I	510	GLN
1	J	431	TYR
1	J	513	ASN
1	J	524	ARG
1	J	675	ILE
1	J	778	LEU
1	J	781	THR
1	J	957	PHE
1	J	999	TYR
2	C	295	VAL
2	C	401	TYR
2	C	564	TYR
2	C	623	ASN
2	B	279	SER
2	B	295	VAL
2	B	309	THR

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Mol	Chain	Res	Type
2	B	369	LEU
2	B	537	LYS
2	B	619	GLN
2	B	658	CYS
1	A	415	SER
1	A	428	LEU
1	A	431	TYR
1	A	513	ASN
1	A	524	ARG
1	A	614	ILE
1	A	879	TYR
1	A	923	ILE
1	A	957	PHE
1	A	982	ASP
1	A	990	LYS
1	A	999	TYR
1	A	1073	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	G	1007	GLN
1	G	1015	HIS
2	L	238	GLN
2	L	618	HIS
2	K	425	ASN
2	E	353	ASN
2	E	583	ASN
2	F	353	ASN
2	F	618	HIS
2	F	619	GLN
1	D	629	GLN
1	D	639	ASN
1	D	641	ASN
2	H	353	ASN
2	H	408	GLN
2	H	485	ASN
2	I	583	ASN
2	I	657	ASN
1	J	1032	GLN
2	C	623	ASN
2	C	657	ASN

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Mol	Chain	Res	Type
2	B	420	ASN
2	B	445	HIS
2	B	485	ASN
2	B	489	ASN
2	B	632	HIS
1	A	348	ASN
1	A	418	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 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

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	701/776 (90%)	-0.14	5 (0%) 87 82	86, 110, 163, 211	0
1	D	683/776 (88%)	-0.13	8 (1%) 79 71	89, 128, 188, 213	0
1	G	683/776 (88%)	-0.14	5 (0%) 87 82	81, 108, 195, 233	0
1	J	681/776 (87%)	-0.16	6 (0%) 84 77	91, 118, 146, 174	0
2	B	429/465 (92%)	-0.22	2 (0%) 90 86	66, 111, 155, 177	0
2	C	444/465 (95%)	-0.12	3 (0%) 87 82	72, 114, 151, 172	0
2	E	414/465 (89%)	-0.26	2 (0%) 90 86	67, 109, 139, 161	0
2	F	442/465 (95%)	-0.20	1 (0%) 94 93	86, 104, 125, 136	0
2	H	420/465 (90%)	-0.31	1 (0%) 94 93	73, 103, 141, 160	0
2	I	437/465 (93%)	-0.19	3 (0%) 87 82	80, 112, 146, 161	0
2	K	431/465 (92%)	-0.13	7 (1%) 72 62	80, 116, 151, 168	0
2	L	441/465 (94%)	-0.27	0 100 100	80, 99, 127, 156	0
All	All	6206/6824 (90%)	-0.18	43 (0%) 87 82	66, 112, 160, 233	0

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	1036	THR	4.8
2	K	246	LEU	4.3
2	B	226	HIS	4.2
2	K	277	PHE	3.9
1	A	716	CYS	3.5
2	F	489	ASN	3.2
2	C	279	SER	3.0
1	D	456	THR	2.9
2	K	248	PRO	2.8
2	K	244	SER	2.8
1	D	676	SER	2.8

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Mol	Chain	Res	Type	RSRZ
1	G	914	VAL	2.7
2	I	331	ASP	2.6
1	D	455	ILE	2.6
1	G	961	TYR	2.5
1	G	456	THR	2.4
1	A	607	ASP	2.4
1	A	1084	HIS	2.4
1	D	662	HIS	2.4
1	A	715	THR	2.4
1	J	787	TYR	2.3
2	E	277	PHE	2.3
2	C	314	PHE	2.2
1	J	760	PHE	2.2
2	E	278	PRO	2.2
2	I	291	TYR	2.2
2	H	311	PHE	2.2
1	D	663	TYR	2.2
1	J	666	THR	2.1
1	D	901	PRO	2.1
2	K	397	ILE	2.1
2	B	229	LEU	2.1
1	J	457	SER	2.1
1	D	721	THR	2.1
1	G	1049	LEU	2.1
2	K	283	VAL	2.1
1	J	536	CYS	2.0
2	I	292	PHE	2.0
1	D	723	THR	2.0
1	J	456	THR	2.0
1	A	940	ALA	2.0
2	C	346	TRP	2.0
2	K	247	LYS	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.