



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 03:03 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

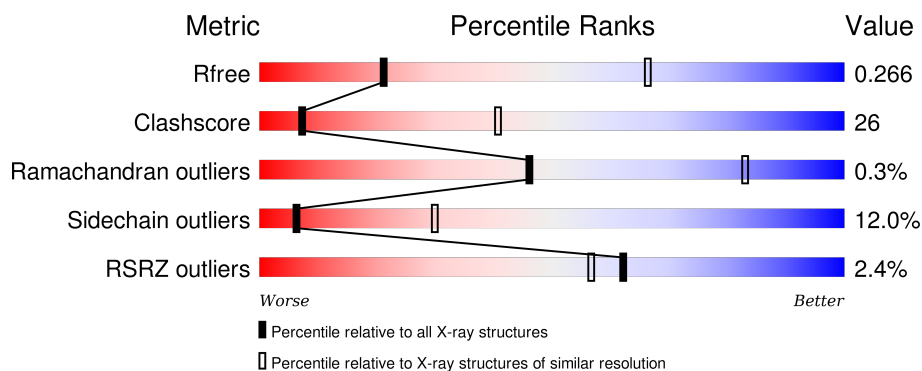
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.41 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.





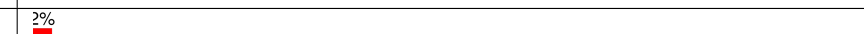



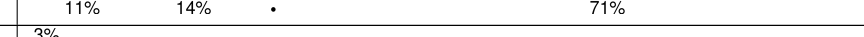
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1049 (3.52-3.32)
Clashscore	102246	1032 (3.50-3.34)
Ramachandran outliers	100387	1002 (3.50-3.34)
Sidechain outliers	100360	1003 (3.50-3.34)
RSRZ outliers	91569	1054 (3.52-3.32)

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

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Mol	Chain	Length	Quality of chain
2	G	249	
2	H	249	
2	I	249	
3	D	727	
3	J	727	
3	K	727	
3	L	727	

2 Entry composition

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
1	A	267	Total	C	N	O	S	0	0	0
			2170	1409	346	404	11			
1	C	267	Total	C	N	O	S	0	0	0
			2174	1412	347	404	11			
1	E	267	Total	C	N	O	S	0	0	0
			2174	1411	347	405	11			
1	F	267	Total	C	N	O	S	0	0	0
			2170	1409	346	404	11			

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

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

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

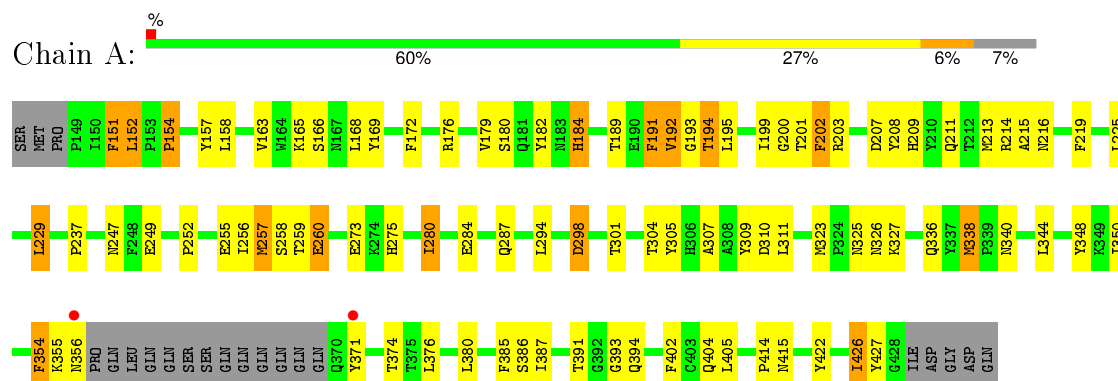
- Molecule 3 is a protein called GLUCOSE-REPRESSIBLE ALCOHOL DEHYDROGENASE TRANSCRIPTIONAL EFFECTOR.

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

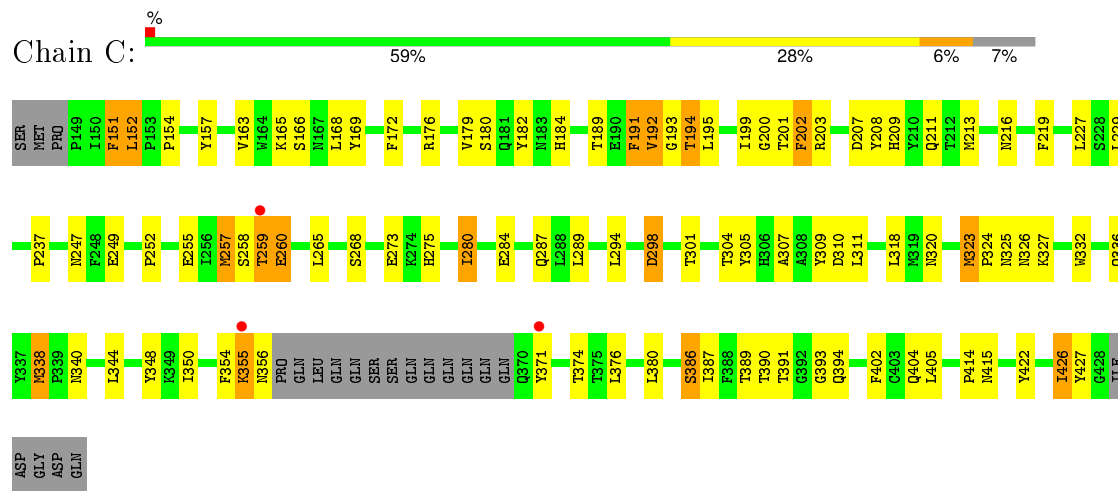
3 Residue-property plots [\(i\)](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

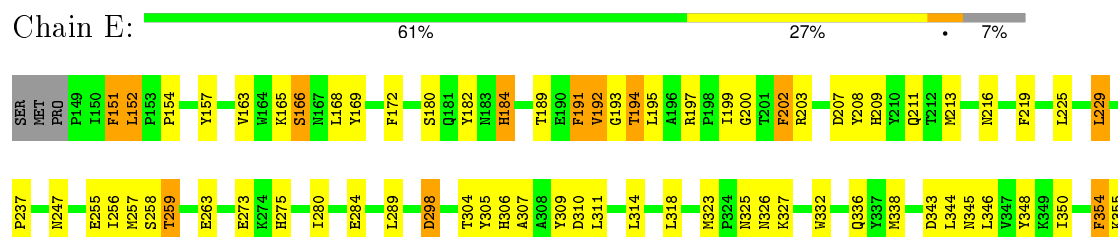
• Molecule 1: POLY(A) RIBONUCLEASE POP2

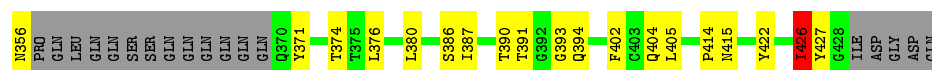


• Molecule 1: POLY(A) RIBONUCLEASE POP2



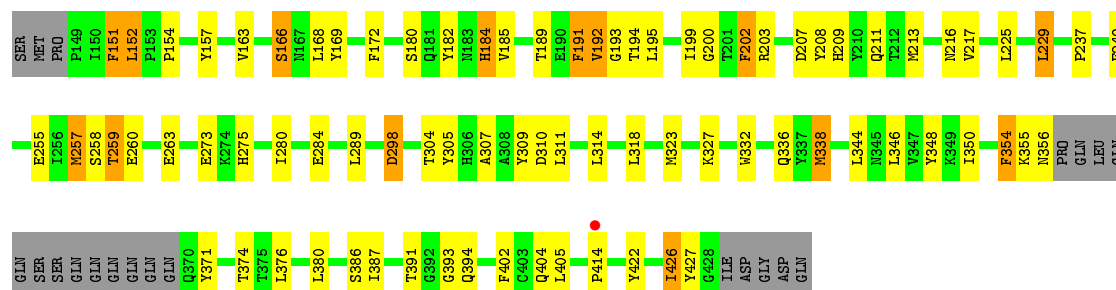
• Molecule 1: POLY(A) RIBONUCLEASE POP2





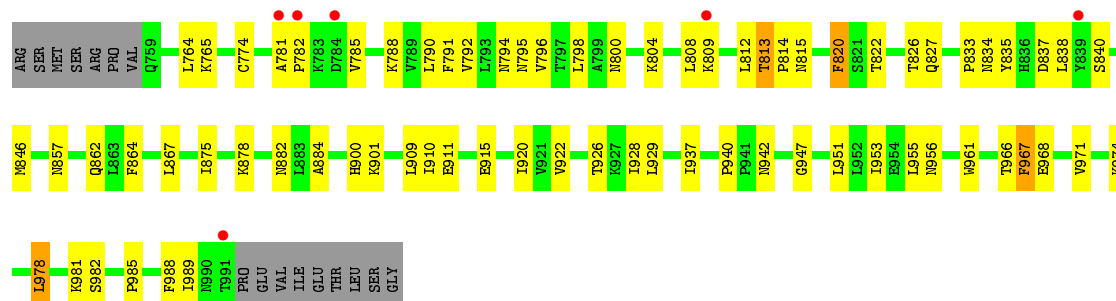
• Molecule 1: POLY(A) RIBONUCLEASE POP2

Chain F: 64% 24% 5% 7%



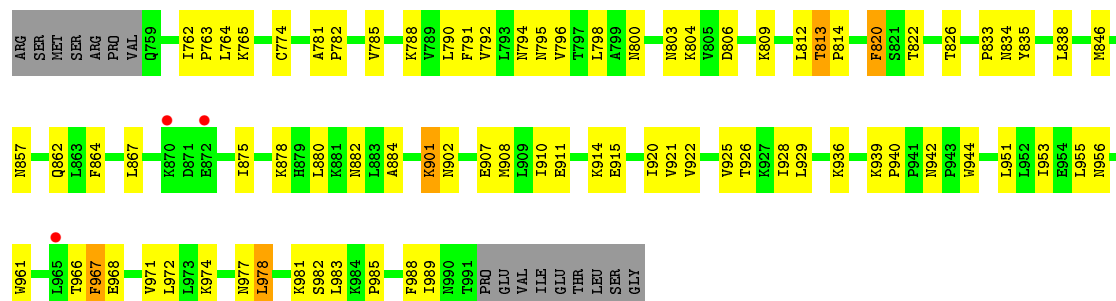
• Molecule 2: GENERAL NEGATIVE REGULATOR OF TRANSCRIPTION SUBUNIT 1

Chain B: 2% 65% 27% 6%



• Molecule 2: GENERAL NEGATIVE REGULATOR OF TRANSCRIPTION SUBUNIT 1

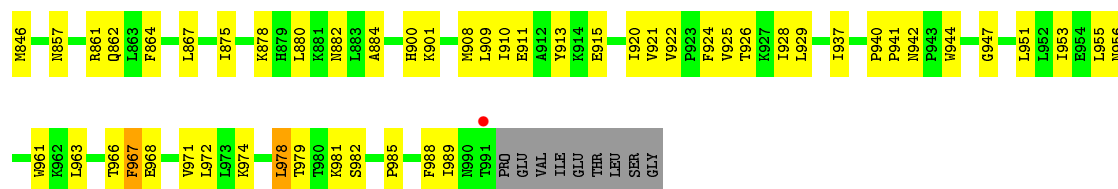
Chain G: 61% 30% 6%



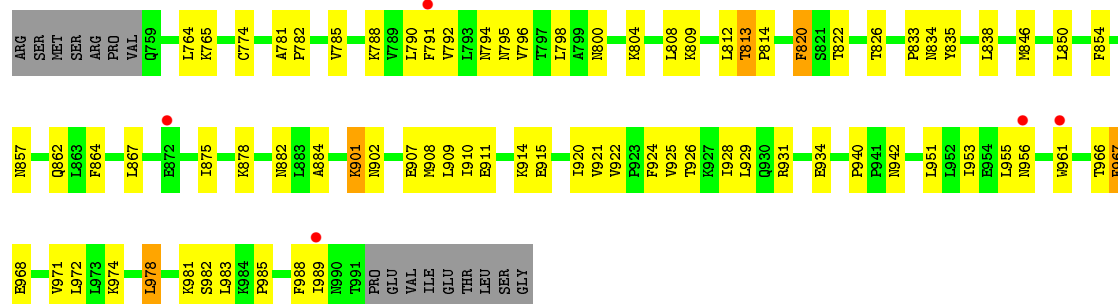
• Molecule 2: GENERAL NEGATIVE REGULATOR OF TRANSCRIPTION SUBUNIT 1

Chain H: 2% 61% 31% 6%

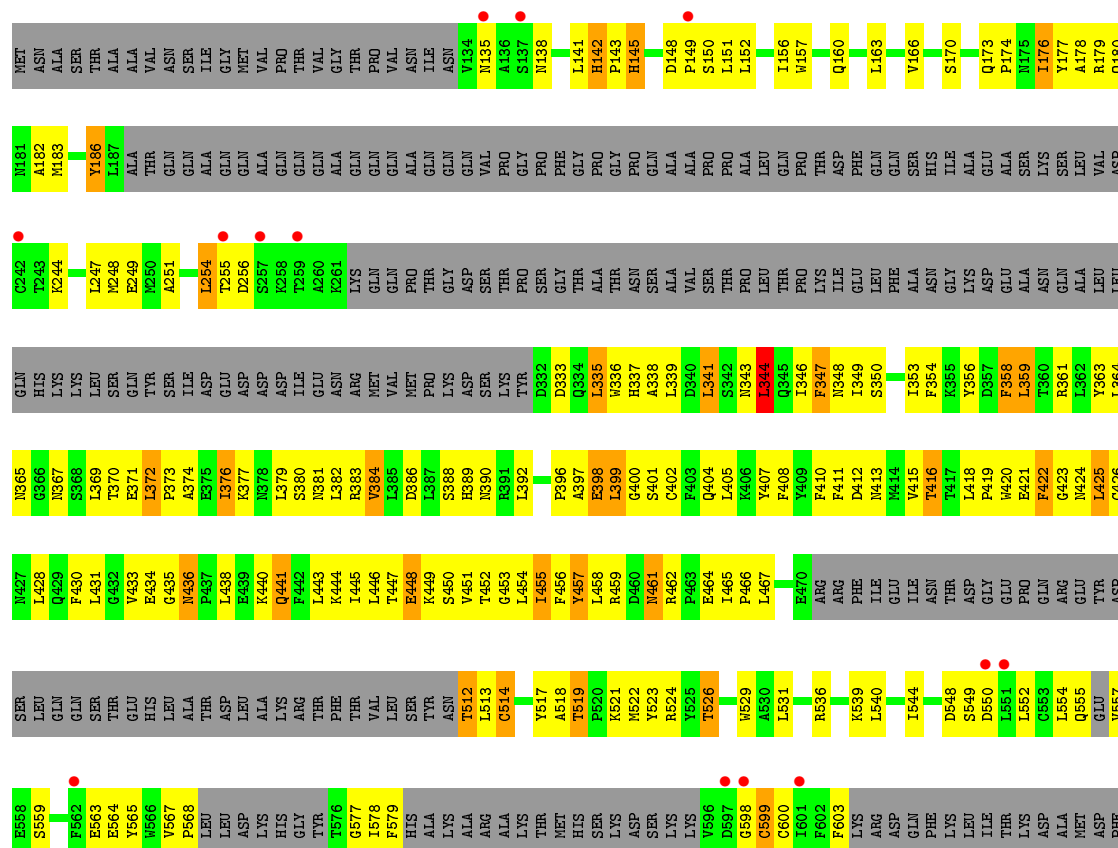


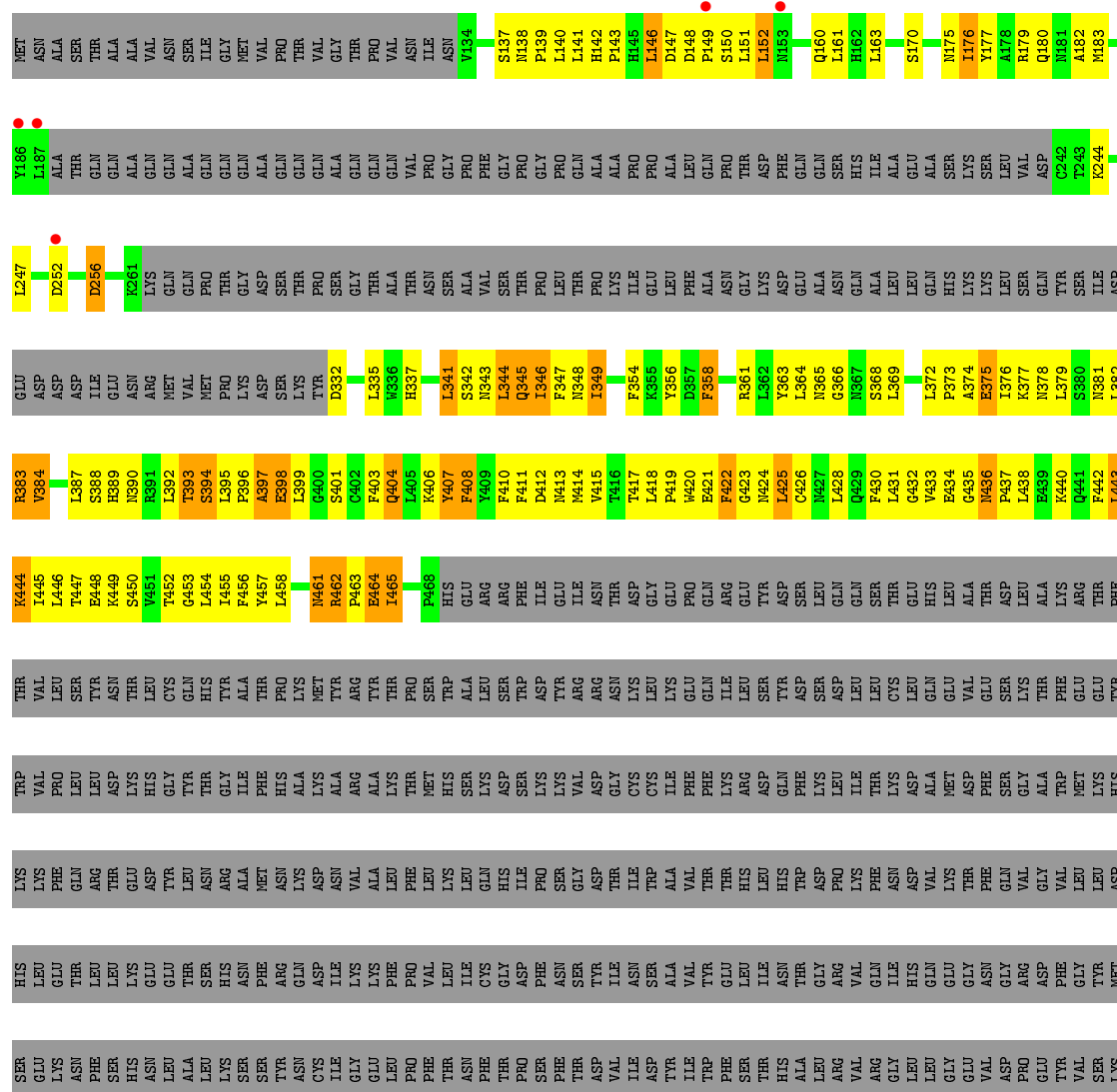


• Molecule 2: GENERAL NEGATIVE REGULATOR OF TRANSCRIPTION SUBUNIT 1

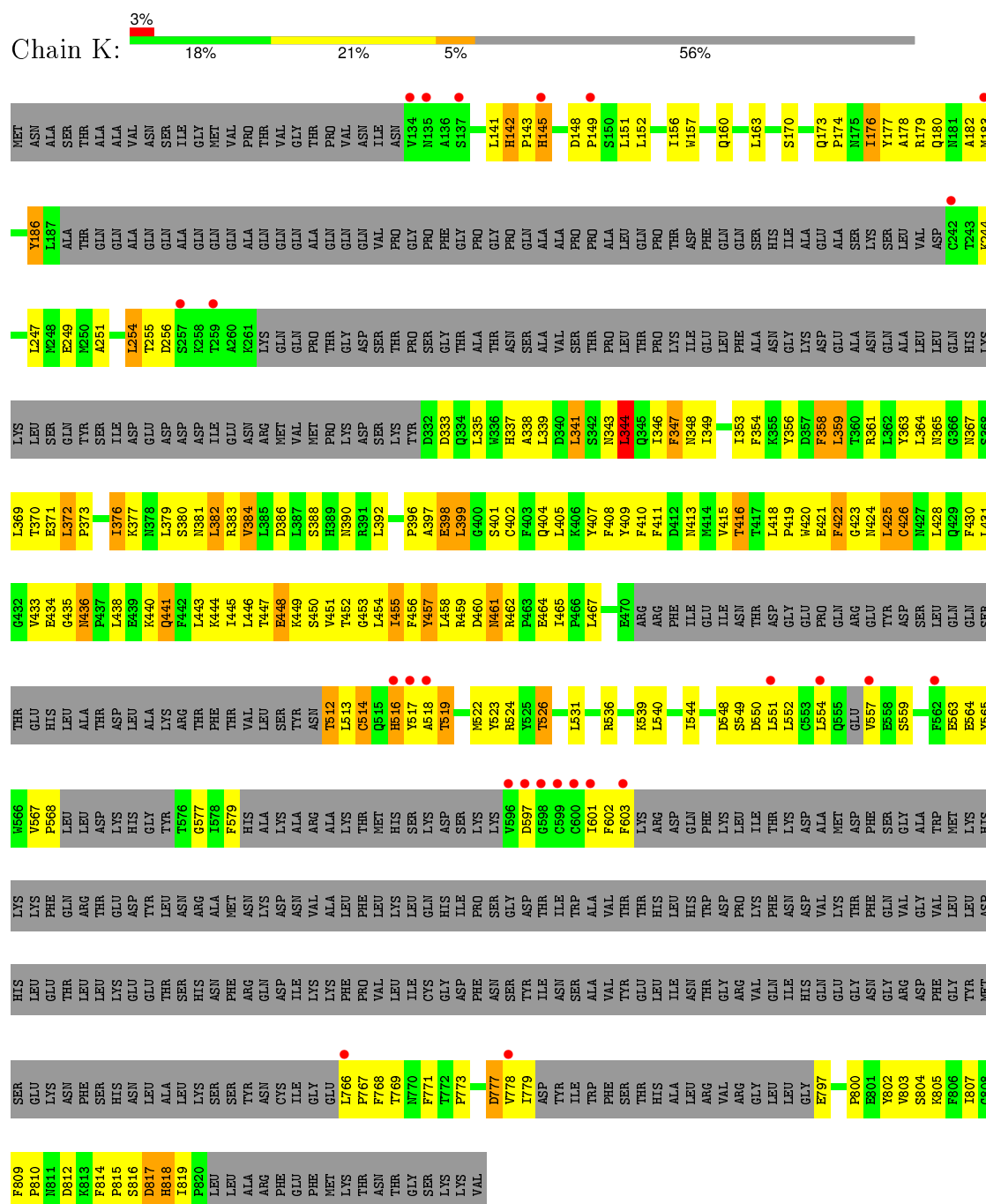


• Molecule 3: GLUCOSE-REPRESSIBLE ALCOHOL DEHYDROGENASE TRANSCRIPTIONAL EFFECTOR





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VAL	SER	GLY	LEU	MET	GLU	ARG	F442	S380	ASP	D246	ASN	MET
LYS	PHE	MET	ASP	HIS	GLU	THR	L443	N381	GLU	L247	ALA	THR
ILE	GLU	SER	HIS	LYS	TRP	THR	K444	L382	ASP	D252	THR	GLN
GLY	ILE	GLU	LEU	LYS	VAL	VAL	I446	R383	ASP	D266	ALA	ALA
PHE	ASN	ASN	THR	PHE	PRO	LEU	T447	S384	ILE	K261	GLN	GLN
PRO	PRO	PHE	LEU	ARG	LEU	SER	E448	L387	GLU	L261	ALA	ALA
ASN	ASN	THR	LEU	THR	LEU	THR	K449	S388	ASN	K261	GLN	GLN
SER	SER	LEU	LEU	THR	ASP	ASN	S450	H389	ARG	LYS	GLN	GLN
ASN	ASN	LYS	LYS	GLU	LYS	THR	T451	L392	MET	GLN	ILE	ILE
LEU	LEU	GLY	GLU	ASP	HIS	LEU	T452	T393	VAL	GLN	GLY	GLY
PRO	PRO	ALA	THR	THR	GLN	CYS	G453	S394	PRO	PRO	GLN	GLN
SER	SER	LEU	SER	ASN	THR	GLN	L454	L395	PRO	THR	MET	MET
ASP	ASP	LYS	HIS	ARG	GLY	THR	L455	L396	LYS	GLY	VAL	VAL
HIS	HIS	SER	ASN	ARG	THR	THR	F456	P396	ASP	ASP	THR	THR
ILE	ILE	SER	ASN	ALA	ILE	ALA	Y457	A397	SER	SER	VAL	VAL
PRO	PRO	THR	PHE	MET	PHE	THR	L458	E398	LYS	THR	GLN	GLN
LEU	LEU	ARG	ARG	ASN	HIS	PRO	L399	L399	THR	PRO	ALA	GLY
LEU	LEU	ASN	GLN	LYS	ALA	LYS	G400	D332	THR	SER	GLN	THR
LEU	LEU	CYS	ASP	ASP	LYS	MET	R461	D333	GLY	SER	GLN	PRO
ALA	ALA	ILE	ILE	ASN	ALA	ALA	P463	L335	THR	THR	GLN	VAL
ARG	ARG	LYS	LYS	VAL	ARG	ARG	F403	L336	ALA	ALA	VAL	ASN
PHE	PHE	GLU	LYS	ALA	ALA	THR	Q404	W336	THR	THR	PRO	ILE
GLU	GLU	LEU	LYS	ALA	ALA	THR	I465	H337	ASN	ASN	GLY	ASN
PRO	PRO	PRO	PHE	LEU	LYS	THR	P466	A338	PRO	PRO	GLY	GLY
PHE	PHE	THR	VAL	PHE	THR	SER	L467	K406	SER	SER	PRO	GLY
THR	THR	ASN	LEU	LEU	MET	SER	P468	Y407	ALA	ALA	PHE	PHE
ASN	ASN	LYS	LEU	LYS	THR	ALA	HIS	D340	VAL	VAL	GLY	GLY
ASN	ASN	CYS	THR	LEU	LEU	ALA	Y409	L341	SER	SER	PRO	PRO
PHE	PHE	GLY	CYS	GLN	LYS	LEU	F410	S342	THR	THR	GLY	GLY
THR	THR	THR	ASP	HIS	ASP	SER	F411	N343	PRO	PRO	PRO	PRO
GLY	GLY	PRO	ASP	ILE	SER	TRP	D412	L344	LEU	LEU	GLN	GLN
SER	SER	PHE	PHE	PRO	LYS	ASP	N413	Q345	THR	THR	ALA	ALA
PHE	PHE	GLY	SER	GLY	LYS	THR	M414	I346	PRO	PRO	ALA	ALA
LYS	LYS	THR	SER	GLY	VAL	ARG	V415	F347	LYS	LYS	PRO	PRO
VAL	VAL	ASP	THR	ASP	ASP	ARG	T416	N348	ILE	ILE	PRO	PRO
VAL	VAL	VAL	ILE	THR	GLY	ASN	T417	I349	GLU	GLU	ALA	ALA
ILE	ILE	ASN	ASN	ILE	CYS	THR	L418	L349	LEU	LEU	LEU	LEU
ASP	ASP	SER	SER	TRP	CYS	LEU	K354	F354	PHE	PHE	GLN	GLN
TYR	TYR	ALA	ALA	ALA	ILE	LYS	W420	N355	ALA	ALA	SER	SER
TRP	TRP	VAL	VAL	VAL	PHE	GLU	Q421	Y356	ASN	ASN	THR	THR
ILE	ILE	THR	THR	THR	THR	GLN	F422	D357	GLY	GLY	ASP	ASP
PHE	PHE	THR	THR	THR	LYS	ILE	G423	F358	LYS	LYS	PHE	PHE
SER	SER	LEU	LEU	HIS	ARG	LEU	M424	L361	ASP	ASP	GLN	GLN
THR	THR	ILE	ILE	LEU	ASP	SER	L425	L362	GLU	GLU	GLN	GLN
HIS	HIS	ASN	ASN	HIS	THR	THR	C426	Y363	ALA	ALA	SER	SER
ALA	ALA	THR	THR	TRP	PHE	THR	N427	L364	ASN	ASN	HIS	HIS

4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ ¹	1.29 (at 3.25Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.7.1_743)	Depositor
R, R_{free}	0.233 , 0.270 0.229 , 0.266	Depositor DCC
R_{free} test set	4463 reflections (5.26%)	DCC
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
Estimated twinning fraction	0.026 for -h,-k,l 0.018 for k,h,-l 0.022 for -k,-h,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 98830 reflections	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	0.56	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(°)	Ideal(°)
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

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:L:422:PHE:CB	3:L:425:LEU:HG	2.02	0.89
3:K:445:ILE:O	3:K:449:LYS:HB2	1.73	0.89
3:J:422:PHE:CD1	3:J:422:PHE:O	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
3:J:422:PHE:CB	3:J:425:LEU:HG	2.04	0.88
1:E:197:ARG:CG	3:L:175:ASN:HD22	1.84	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:O	3:K:579:PHE:HD1	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
3:L:170:SER:HB3	3:L:176:ILE:HD13	1.63	0.80
1:A:169:TYR:OH	1:A:284:GLU:OE1	1.99	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:K:418:LEU:HB3	3:K:422:PHE:HE1	1.47	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: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
3:D:372:LEU:HD21	3:D:376:ILE:HD13	1.68	0.76
1:A:203:ARG:HH22	3:D:333:ASP:CB	1.99	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
3:J:422:PHE:HB3	3:J:425:LEU:HG	1.66	0.75
2:I:790:LEU:O	2:I:794:ASN:ND2	2.19	0.75
1:A:189:THR:OG1	1:A:310:ASP:OD1	2.04	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
3:J:422:PHE:HB2	3:J:425:LEU:HG	1.69	0.73
1:E:203:ARG:HH22	3:L:333:ASP:CB	2.00	0.73
3:D:397:ALA:O	3:D:398:GLU:HG2	1.88	0.73
3:L:422:PHE:HB3	3:L:425:LEU:HG	1.68	0.73
1:F:202:PHE:CE2	1:F:208:TYR:CD1	2.76	0.73
1:F:189:THR:OG1	1:F:310:ASP:OD1	2.05	0.73
3:J:442:PHE:HE1	3:J:458:LEU:HD21	1.53	0.73
3:K:428:LEU:HD21	3:K:431:LEU:HB2	1.69	0.73
1:E:195:LEU:HA	1:E:216:ASN:OD1	1.88	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
3:K:422:PHE:HB2	3:K:425:LEU:HD11	1.70	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

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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:K:372:LEU:HD21	3:K:376:ILE:HD13	1.71	0.72
3:D:766:LEU:CG	3:D:767:PRO:HD2	2.18	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
3:K:422:PHE:HB3	3:K:425:LEU:CG	2.19	0.71
1:E:191:PHE:CZ	1:E:309:TYR:HD2	2.06	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
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: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:K:411:PHE:HD1	3:K:434:GLU:O	1.74	0.71
1:C:176:ARG:HD3	2:H:900:HIS:HB3	1.73	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:N	3:K:461:ASN:OD1	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:419:PRO:O	3:L:420:TRP:HB2	1.92	0.69
3:L:383:ARG:NH1	3:L:404:GLN:HG2	2.06	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
1:C:195:LEU:HA	1:C:216:ASN:OD1	1.91	0.69
3:L:397:ALA:O	3:L:398:GLU:HG2	1.93	0.69
3:L:433:VAL:O	3:L:435:GLY:HA2	1.91	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:579:PHE:CZ	3:D:598:GLY:HA3	2.27	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
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
1:C:213:MET:HG3	1:C:309:TYR:CD1	2.28	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:K:446:LEU:HD12	3:K:450:SER:O	1.95	0.66
3:J:347:PHE:HD1	3:J:368:SER:HB2	1.59	0.66
1:A:176:ARG:HD3	2:B:900:HIS:HB3	1.77	0.66
3:L:244:LYS:O	3:L:247:LEU:N	2.28	0.66
3:D:335:LEU:O	3:D:337:HIS:CE1	2.49	0.66
2:H:781:ALA:HB1	2:H:785:VAL:HB	1.78	0.66
3:K:361:ARG:HA	3:K:384:VAL:HG23	1.78	0.65
3:K:335:LEU:O	3:K:337:HIS:CE1	2.49	0.65
3:J:396:PRO:HD2	3:J:399:LEU:HD12	1.77	0.65
3:D:397:ALA:C	3:D:399:LEU:H	1.99	0.65
3:D:142:HIS:H	3:D:142:HIS:CD2	2.12	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
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
1:E:194:THR:O	1:E:194:THR:HG23	1.97	0.65
3:K:540:LEU:HD23	3:K:815:PRO:HG2	1.79	0.65
3:J:346:ILE:HG22	3:J:346:ILE:O	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
2:I:967:PHE:O	2:I:971:VAL:HG23	1.97	0.64
3:D:251:ALA:O	3:D:254:LEU:N	2.29	0.64
3:L:420:TRP:CE2	3:L:463:PRO:HD3	2.32	0.64
3:D:346:ILE:HB	3:D:367:ASN:HD22	1.63	0.64
1:A:213:MET:HG3	1:A:309:TYR:CD1	2.32	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
1:A:287:GLN:HE22	2:B:947:GLY:HA3	1.62	0.64
3:J:419:PRO:HD2	3:J:422:PHE:HE1	1.62	0.64
3:D:157:TRP:HZ3	3:D:443:LEU:HD22	1.62	0.64
1:A:305:TYR:HD1	1:A:344:LEU:HB3	1.61	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
3:K:397:ALA:C	3:K:399:LEU:H	2.01	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:J:433:VAL:O	3:J:435:GLY:HA2	1.98	0.63
3:L:440:LYS:HA	3:L:443:LEU:HB2	1.79	0.63
3:K:183:MET:O	3:K:186:TYR:HB3	1.98	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
3:D:766:LEU:CD1	3:D:767:PRO:HD2	2.29	0.63
1:C:191:PHE:HD1	1:C:191:PHE:N	1.96	0.63
3:K:550:ASP:O	3:K:603:PHE:HA	1.98	0.63
3:L:417:THR:HG23	3:L:442:PHE:CE2	2.34	0.63
3:K:513:LEU:HD12	3:K:816:SER:HA	1.80	0.63
3:D:518:ALA:O	3:D:531:LEU:HD11	1.97	0.63
3:D:183:MET:O	3:D:186:TYR:HB3	1.98	0.63
1:F:191:PHE:HD1	1:F:191:PHE:N	1.96	0.63
3:J:403:PHE:CD1	3:J:404:GLN:N	2.67	0.63
2:B:875:ILE:HD12	2:B:920:ILE:HG12	1.79	0.63
2:I:781:ALA:HB1	2:I:785:VAL:HB	1.78	0.63
1:C:355:LYS:HG3	1:C:355:LYS:O	1.97	0.63
2:I:956:ASN:HD21	2:I:966:THR:HG23	1.63	0.62
3:D:540:LEU:HD23	3:D:815:PRO:HG2	1.81	0.62
1:C:202:PHE:CE2	1:C:208:TYR:CD1	2.85	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:884:ALA:HB1	2:B:928:ILE:HG13	1.81	0.62
3:K:766:LEU:CD1	3:K:767:PRO:HD2	2.30	0.62
2:B:781:ALA:HB1	2:B:785:VAL:HB	1.82	0.62
3:D:179:ARG:O	3:D:182:ALA:HB3	1.99	0.62
1:E:197:ARG:HG3	3:L:175:ASN:HD22	1.63	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
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
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
2:B:967:PHE:O	2:B:971:VAL:HG23	2.00	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
3:D:433:VAL:O	3:D:435:GLY:HA2	2.00	0.61
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:L:403:PHE:CD1	3:L:404:GLN:N	2.69	0.61
1:A:192:VAL:HG11	1:A:257:MET:HG2	1.82	0.61
3:K:420:TRP:CZ3	3:K:461:ASN:O	2.54	0.61
1:C:191:PHE:CD1	1:C:191:PHE:N	2.67	0.61
1:F:305:TYR:HD1	1:F:344:LEU:HB3	1.63	0.61
1:F:195:LEU:HA	1:F:216:ASN:OD1	2.01	0.61
3:K:449:LYS:HB3	3:K:453:GLY:HA3	1.83	0.61
2:I:884:ALA:HB1	2:I:928:ILE:HG13	1.82	0.61
1:F:154:PRO:HG2	1:F:157:TYR:CD1	2.36	0.61
3:L:379:LEU:O	3:L:382:LEU:HB2	2.01	0.61
2:H:967:PHE:O	2:H:971:VAL:HG23	2.01	0.61
1:F:192:VAL:HG11	1:F:257:MET:HG2	1.83	0.61
3:J:396:PRO:O	3:J:399:LEU:HB2	2.00	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:K:419:PRO:HD2	3:K:422:PHE:CZ	2.36	0.61
3:K:251:ALA:O	3:K:254:LEU:N	2.33	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
3:L:396:PRO:O	3:L:399:LEU:HB2	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:875:ILE:HD12	2:H:920:ILE:HG12	1.81	0.60
3:K:512:THR:O	3:K:512:THR:CG2	2.48	0.60
2:I:922:VAL:O	2:I:926:THR:HG23	2.02	0.60
3:J:345:GLN:OE1	3:J:345:GLN:N	2.34	0.60
1:E:191:PHE:N	1:E:191:PHE:HD1	1.99	0.60
3:K:420:TRP:O	3:K:422:PHE:O	2.19	0.60
3:K:349:ILE:HD11	3:K:369:LEU:HD21	1.83	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:H	1:F:191:PHE:HD1	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
3:K:440:LYS:HA	3:K:443:LEU:HD12	1.84	0.59
2:B:782:PRO:HG2	2:B:785:VAL:HG23	1.82	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
3:D:578:ILE:HD12	3:D:578:ILE:N	2.17	0.59
3:D:411:PHE:CD1	3:D:434:GLU:O	2.55	0.59
2:B:956:ASN:HD21	2:B:966:THR:HG23	1.66	0.59
3:D:424:ASN:ND2	3:D:807:ILE:HG21	2.11	0.59
3:D:346:ILE:HB	3:D:367:ASN:ND2	2.17	0.59
1:A:202:PHE:CE2	1:A:208:TYR:CD1	2.89	0.59
3:D:769:THR:HG23	3:D:778:VAL:HG13	1.83	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
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
1:E:202:PHE:CE1	3:L:336:TRP:HB3	2.38	0.58
1:F:191:PHE:HZ	1:F:309:TYR:HD2	1.51	0.58
1:C:151:PHE:C	1:C:151:PHE:CD1	2.76	0.58
3:D:768:PHE:CE2	3:D:771:PHE:HB2	2.38	0.58
3:D:512:THR:O	3:D:512:THR:CG2	2.51	0.58
2:H:956:ASN:HD21	2:H:966:THR:HG23	1.66	0.58
3:K:422:PHE:HB2	3:K:425:LEU:CD1	2.31	0.58
1:A:191:PHE:HD1	1:A:191:PHE:N	2.01	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:199:ILE:HB	3:D:338:ALA:HB3	1.84	0.58
3:L:177:TYR:CD2	3:L:363:TYR:CZ	2.91	0.58
3:K:516:HIS:ND1	3:K:516:HIS:O	2.37	0.58
2:B:953:ILE:HG22	2:B:985:PRO:HB3	1.86	0.58
3:D:423:GLY:H	3:D:458:LEU:HB2	1.67	0.58
3:K:347:PHE:H	3:K:347:PHE:HD1	1.50	0.58
2:G:834:ASN:HB2	2:G:835:TYR:CD1	2.39	0.58
3:J:428:LEU:HD21	3:J:431:LEU:HB2	1.85	0.58
3:L:422:PHE:CB	3:L:425:LEU:CG	2.80	0.58
3:J:417:THR:HG23	3:J:442:PHE:CE2	2.39	0.58
3:L:179:ARG:O	3:L:182:ALA:HB3	2.04	0.58
2:B:955:LEU:HD23	2:B:989:ILE:HG13	1.85	0.58
3:K:539:LYS:CB	3:K:815:PRO:HG3	2.33	0.58
3:K:148:ASP:HB3	3:K:149:PRO:C	2.24	0.58
2:H:955:LEU:HD23	2:H:989:ILE:HG13	1.85	0.58
1:E:191:PHE:HZ	1:E:309:TYR:HD2	1.51	0.58
1:A:298:ASP:N	1:A:298:ASP:OD1	2.35	0.58
3:K:512:THR:O	3:K:512:THR:HG23	2.04	0.58
3:J:177:TYR:CD2	3:J:363:TYR:CZ	2.92	0.58
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:D:455:ILE:HG22	3:D:456:PHE:N	2.19	0.57
3:K:766:LEU:HD12	3:K:767:PRO:HD2	1.86	0.57
1:A:191:PHE:CD1	1:A:191:PHE:N	2.72	0.57
1:E:191:PHE:N	1:E:191:PHE:CD1	2.70	0.57
3:D:802:TYR:O	3:D:804:SER:O	2.21	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
2:G:800:ASN:ND2	2:G:804:LYS:HG3	2.20	0.57
1:C:199:ILE:HG22	1:C:200:GLY:H	1.69	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
1:C:191:PHE:HD1	1:C:191:PHE:H	1.51	0.57
1:A:257:MET:O	3:D:347:PHE:CD1	2.58	0.57
1:A:151:PHE:C	1:A:151:PHE:CD1	2.78	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:J:419:PRO:O	3:J:421:GLU:HG2	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:539:LYS:CB	3:D:815:PRO:HG3	2.34	0.57
3:L:140:LEU:HG	3:L:437:PRO:HB3	1.86	0.57
3:K:179:ARG:O	3:K:182:ALA:HB3	2.05	0.56
3:D:422:PHE:CA	3:D:424:ASN:H	2.18	0.56
3:K:422:PHE:CD2	3:K:425:LEU:HD21	2.41	0.56
3:K:143:PRO:HD2	3:K:157:TRP:CH2	2.40	0.56
3:K:369:LEU:HD13	3:K:390:ASN:OD1	2.05	0.56
2:H:812:LEU:HD21	2:H:820:PHE:HD2	1.70	0.56
3:J:396:PRO:C	3:J:397:ALA:O	2.37	0.56
3:D:148:ASP:HB3	3:D:149:PRO:C	2.25	0.56
3:K:436:ASN:O	3:K:438:LEU:N	2.38	0.56
1:E:191:PHE:H	1:E:191:PHE:HD1	1.52	0.56
1:F:151:PHE:CD1	1:F:151:PHE:C	2.75	0.56
3:D:444:LYS:HB3	2:H:963:LEU:HD12	1.87	0.56
1:A:257:MET:O	3:D:347:PHE:HD1	1.88	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
3:J:397:ALA:O	3:J:398:GLU:CG	2.53	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
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
3:L:422:PHE:HB2	3:L:425:LEU:CG	2.34	0.56
1:F:194:THR:O	1:F:194:THR:CG2	2.52	0.56
1:F:193:GLY:C	1:F:195:LEU:HD23	2.26	0.56
1:C:199:ILE:HB	3:K:338:ALA:HB3	1.87	0.56
3:D:523:TYR:N	3:D:523:TYR:CD1	2.72	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:N	1:E:354:PHE:HD1	2.04	0.55
3:K:768:PHE:CE2	3:K:771:PHE:HB2	2.42	0.55
3:K:381:ASN:O	3:K:383:ARG:NH1	2.39	0.55
1:A:207:ASP:O	1:A:211:GLN:HG2	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:160:GLN:NE2	3:K:430:PHE:CE1	2.73	0.55
2:G:875:ILE:HD12	2:G:920:ILE:HG12	1.88	0.55
3:J:419:PRO:CD	3:J:422:PHE:CE1	2.89	0.55
1:E:213:MET:HG3	1:E:309:TYR:CE1	2.41	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
3:L:419:PRO:HD2	3:L:422:PHE:CZ	2.40	0.55
3:K:423:GLY:H	3:K:458:LEU:HB2	1.71	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
1:E:354:PHE:HD2	1:E:414:PRO:HB2	1.72	0.55
1:E:151:PHE:CD1	1:E:151:PHE:C	2.77	0.55
3:D:142:HIS:N	3:D:142:HIS:CD2	2.75	0.55
2:I:782:PRO:HG2	2:I:785:VAL:HG23	1.87	0.55
3:D:436:ASN:O	3:D:438:LEU:N	2.39	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
2:G:955:LEU:HD23	2:G:989:ILE:HG13	1.88	0.55
3:J:421:GLU:C	3:J:424:ASN:HB2	2.27	0.55
3:D:369:LEU:HD13	3:D:390:ASN:OD1	2.07	0.55
1:C:344:LEU:HD13	1:C:402:PHE:HB2	1.88	0.55
1:F:354:PHE:HD1	1:F:354:PHE:N	2.05	0.55
1:A:354:PHE:N	1:A:354:PHE:HD1	2.04	0.55
3:K:174:PRO:O	3:K:179:ARG:NH2	2.39	0.55
3:D:143:PRO:HD2	3:D:157:TRP:CH2	2.42	0.55
3:K:415:VAL:H	3:K:436:ASN:HB3	1.72	0.55
3:D:512:THR:HG23	3:D:512:THR:O	2.07	0.55
2:H:951:LEU:HD13	2:H:988:PHE:HD2	1.72	0.55
1:E:154:PRO:HG2	1:E:157:TYR:CD1	2.42	0.55
1:F:344:LEU:HD13	1:F:402:PHE:HB2	1.89	0.55
1:F:213:MET:HG3	1:F:309:TYR:CE1	2.42	0.55
1:A:387:ILE:O	1:A:393:GLY:HA3	2.07	0.55
2:H:798:LEU:HD12	2:H:838:LEU:HD13	1.89	0.55
3:K:346:ILE:HB	3:K:367:ASN:ND2	2.21	0.55
3:D:367:ASN:HB2	3:D:369:LEU:HD13	1.88	0.55
3:D:160:GLN:NE2	3:D:430:PHE:HE1	2.05	0.55
2:I:834:ASN:HB2	2:I:835:TYR:CD1	2.42	0.55
2:I:798:LEU:HD12	2:I:838:LEU:HD13	1.87	0.55
3:J:148:ASP:HB3	3:J:149:PRO:O	2.06	0.54
1:A:354:PHE:N	1:A:354:PHE:CD1	2.73	0.54
3:D:347:PHE:H	3:D:347:PHE:HD1	1.53	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:199:ILE:HG22	1:A:200:GLY:H	1.72	0.54
2:H:834:ASN:HB2	2:H:835:TYR:CD1	2.43	0.54
3:K:443:LEU:O	3:K:447:THR:HG23	2.07	0.54
1:E:348:TYR:CE1	1:E:376:LEU:HD13	2.43	0.54
1:A:191:PHE:CZ	1:A:309:TYR:CD2	2.94	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:424:ASN:ND2	3:K:807:ILE:HG21	2.14	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:J:420:TRP:CE2	3:J:463:PRO:CD	2.89	0.54
3:L:418:LEU:HD11	3:L:454:LEU:HD21	1.90	0.54
3:L:393:THR:HA	3:L:414:MET:O	2.07	0.54
1:E:354:PHE:CD1	1:E:354:PHE:N	2.74	0.54
2:B:826:THR:HG22	2:B:862:GLN:OE1	2.08	0.54
3:D:457:TYR:C	3:D:457:TYR:CD1	2.80	0.54
3:K:416:THR:O	3:K:438:LEU:HD23	2.07	0.54
3:K:367:ASN:HB2	3:K:369:LEU:HD13	1.90	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
2:B:910:ILE:HD11	2:B:988:PHE:HB3	1.88	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:N	2:I:907:GLU:OE1	2.30	0.54
2:B:940:PRO:HA	2:B:942:ASN:H	1.73	0.54
3:K:143:PRO:HD2	3:K:157:TRP:CZ2	2.42	0.54
3:D:381:ASN:O	3:D:383:ARG:NH1	2.41	0.54
3:D:420:TRP:O	3:D:422:PHE:O	2.26	0.54
1:A:354:PHE:HD2	1:A:414:PRO:HB2	1.73	0.54
3:K:457:TYR:C	3:K:457:TYR:CD1	2.81	0.54
1:F:354:PHE:CD1	1:F:354:PHE:N	2.75	0.54
1:F:199:ILE:HG22	1:F:200:GLY:H	1.70	0.54
3:D:341:LEU:HB2	3:D:364:LEU:HD23	1.88	0.54
3:K:817:ASP:N	3:K:817:ASP:OD1	2.37	0.53
3:K:567:VAL:CG1	3:K:568:PRO:CD	2.84	0.53
3:L:421:GLU:C	3:L:424:ASN:HB2	2.29	0.53
3:K:422:PHE:HB3	3:K:425:LEU:CD2	2.38	0.53
1:F:376:LEU:HD11	1:F:405:LEU:HD22	1.89	0.53
2:B:956:ASN:OD1	2:B:966:THR:HG23	2.08	0.53
3:L:138:ASN:HB3	3:L:141:LEU:HD23	1.90	0.53
3:J:140:LEU:HG	3:J:437:PRO:HB3	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:387:ILE:O	1:F:393:GLY:HA3	2.07	0.53
3:J:335:LEU:O	3:J:337:HIS:ND1	2.40	0.53
3:D:152:LEU:HD12	3:D:152:LEU:H	1.72	0.53
3:J:252:ASP:O	3:J:256:ASP:HB2	2.08	0.53
3:D:567:VAL:CG1	3:D:568:PRO:CD	2.84	0.53
1:C:354:PHE:CD1	1:C:354:PHE:N	2.75	0.53
2:B:813:THR:HG22	2:B:814:PRO:HD2	1.91	0.53
3:K:422:PHE:CB	3:K:425:LEU:CG	2.85	0.53
2:H:971:VAL:O	2:H:974:LYS:HB3	2.08	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:I:812:LEU:HD21	2:I:820:PHE:HD2	1.73	0.53
3:K:346:ILE:H	3:K:367:ASN:HB3	1.73	0.53
3:J:393:THR:HA	3:J:414:MET:O	2.07	0.53
3:K:523:TYR:CD1	3:K:523:TYR:N	2.74	0.53
3:J:420:TRP:NE1	3:J:463:PRO:CD	2.72	0.53
2:H:953:ILE:HG22	2:H:985:PRO:HB3	1.91	0.53
2:B:834:ASN:HB2	2:B:835:TYR:CD1	2.44	0.53
1:A:273:GLU:OE1	1:A:273:GLU:N	2.40	0.53
3:D:346:ILE:H	3:D:367:ASN:HB3	1.73	0.53
3:L:148:ASP:HB3	3:L:149:PRO:O	2.08	0.53
3:J:446:LEU:O	3:J:450:SER:HA	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
3:J:397:ALA:HB1	3:J:421:GLU:HG3	1.90	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
1:A:344:LEU:HD21	1:A:376:LEU:HD23	1.91	0.53
2:I:867:LEU:HD23	2:I:920:ILE:HG22	1.91	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:C:354:PHE:HD1	1:C:354:PHE:N	2.05	0.53
1:A:350:ILE:HD11	1:A:422:TYR:CE2	2.44	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
3:J:419:PRO:O	3:J:420:TRP:HB2	2.09	0.52
3:D:376:ILE:O	3:D:379:LEU:HB2	2.09	0.52
3:J:152:LEU:H	3:J:152:LEU:HD12	1.73	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:392:LEU:HD12	3:K:413:ASN:ND2	2.24	0.52
1:A:219:PHE:HE1	3:D:356:TYR:CD1	2.27	0.52
3:J:344:LEU:O	3:J:346:ILE:HB	2.10	0.52
1:A:247:ASN:HB3	1:A:275:HIS:CE1	2.44	0.52
2:I:978:LEU:HB3	2:I:982:SER:OG	2.09	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
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
1:C:350:ILE:HD11	1:C:422:TYR:CE2	2.45	0.52
3:J:438:LEU:HD13	3:J:443:LEU:HD23	1.92	0.52
2:H:812:LEU:HD23	2:H:846:MET:CE	2.40	0.52
3:J:141:LEU:CD1	3:J:437:PRO:HD3	2.40	0.52
2:H:813:THR:HG22	2:H:814:PRO:HD2	1.92	0.52
1:F:289:LEU:HD23	1:F:318:LEU:HD21	1.92	0.52
3:J:410:PHE:N	3:J:410:PHE:CD1	2.77	0.52
1:E:376:LEU:HD11	1:E:405:LEU:HD22	1.91	0.52
1:C:191:PHE:CZ	1:C:309:TYR:CD2	2.97	0.52
3:K:335:LEU:O	3:K:337:HIS:ND1	2.43	0.52
2:H:788:LYS:O	2:H:792:VAL:HG23	2.09	0.52
3:K:451:VAL:HG12	3:K:452:THR:N	2.25	0.52
1:A:191:PHE:HZ	1:A:309:TYR:HD2	1.55	0.52
3:L:407:TYR:N	3:L:407:TYR:CD1	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
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:D:447:THR:O	3:D:448:GLU:CD	2.49	0.51
1:A:376:LEU:HD11	1:A:405:LEU:HD22	1.91	0.51
3:J:403:PHE:HD1	3:J:404:GLN:N	2.09	0.51
1:F:354:PHE:O	1:F:355:LYS:CB	2.58	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
2:I:911:GLU:O	2:I:915:GLU:HG2	2.10	0.51
3:K:145:HIS:ND1	3:K:145:HIS:O	2.44	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:422:PHE:HD2	3:K:425:LEU:HD21	1.74	0.51
3:L:150:SER:CA	3:L:152:LEU:HD12	2.33	0.51
2:B:971:VAL:O	2:B:974:LYS:HB3	2.10	0.51
3:L:446:LEU:O	3:L:450:SER:HA	2.09	0.51
3:L:428:LEU:HD21	3:L:431:LEU:HB2	1.91	0.51
1:A:348:TYR:CE1	1:A:376:LEU:HD13	2.46	0.51
1:E:193:GLY:C	1:E:195:LEU:HD23	2.30	0.51
3:K:434:GLU:OE1	3:K:435:GLY:HA3	2.11	0.51
3:J:411:PHE:O	3:J:412:ASP:CB	2.59	0.51
2:B:812:LEU:HD21	2:B:820:PHE:HD2	1.75	0.51
3:L:422:PHE:HB3	3:L:425:LEU:CG	2.38	0.51
3:L:141:LEU:CD1	3:L:437:PRO:HD3	2.41	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: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
3:D:421:GLU:O	3:D:424:ASN:HB2	2.11	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
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
2:B:798:LEU:HD12	2:B:838:LEU:HD13	1.93	0.51
1:C:194:THR:O	1:C:194:THR:HG23	2.11	0.51
3:D:145:HIS:O	3:D:145:HIS:ND1	2.44	0.51
3:J:407:TYR:N	3:J:407:TYR:CD1	2.79	0.51
2:I:953:ILE:HG22	2:I:985:PRO:HB3	1.92	0.51
1:A:391:THR:O	1:A:394:GLN:HB2	2.11	0.51
3:J:461:ASN:OD1	3:J:461:ASN:N	2.42	0.51
3:L:419:PRO:CD	3:L:422:PHE:CE1	2.93	0.50
1:C:344:LEU:HD21	1:C:376:LEU:HD23	1.93	0.50
3:L:410:PHE:N	3:L:410:PHE:CD1	2.78	0.50
3:D:526:THR:HB	3:D:810:PRO:O	2.11	0.50
3:D:174:PRO:O	3:D:179:ARG:NH2	2.45	0.50
3:L:152:LEU:H	3:L:152:LEU:HD12	1.76	0.50
1:C:252:PRO:HB3	1:C:257:MET:CE	2.41	0.50
3:J:423:GLY:HA2	3:J:455:ILE:HD12	1.93	0.50
1:E:273:GLU:N	1:E:273:GLU:OE1	2.43	0.50
3:K:451:VAL:O	3:K:454:LEU:N	2.44	0.50
1:E:154:PRO:HG2	1:E:157:TYR:CE1	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:461:ASN:N	3:L:461:ASN:OD1	2.44	0.50
1:C:182:TYR:CZ	1:C:237:PRO:HD3	2.46	0.50
3:J:163:LEU:HD12	3:J:430:PHE:CE1	2.46	0.50
3:D:549:SER:HB3	3:D:552:LEU:CD2	2.41	0.50
3:D:422:PHE:CD2	3:D:425:LEU:HD21	2.47	0.50
2:B:951:LEU:HD13	2:B:988:PHE:HD2	1.76	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
3:D:800:PRO:HA	3:D:803:VAL:HG22	1.93	0.50
3:J:444:LYS:HE3	3:J:448:GLU:OE2	2.10	0.50
2:H:826:THR:HG22	2:H:862:GLN:OE1	2.12	0.50
1:A:219:PHE:CE2	3:D:353:ILE:HG22	2.46	0.50
1:C:355:LYS:NZ	1:C:355:LYS:HB2	2.26	0.50
1:C:199:ILE:HD13	3:K:178:ALA:HA	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
1:E:304:THR:HB	1:E:307:ALA:HB2	1.94	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
3:K:559:SER:O	3:K:563:GLU:HG2	2.12	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:L:397:ALA:C	3:L:399:LEU:H	2.15	0.50
3:L:422:PHE:HB2	3:L:425:LEU:CD1	2.42	0.50
1:F:151:PHE:C	1:F:151:PHE:HD1	2.14	0.50
3:L:163:LEU:HD12	3:L:430:PHE:CZ	2.46	0.50
3:D:817:ASP:OD1	3:D:817:ASP:N	2.39	0.50
1:F:273:GLU:OE1	1:F:273:GLU:N	2.44	0.50
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:C:151:PHE:HD1	1:C:151:PHE:C	2.15	0.49
1:C:207:ASP:O	1:C:211:GLN:HG2	2.11	0.49
3:K:428:LEU:HB3	3:K:455:ILE:CD1	2.41	0.49
1:F:298:ASP:N	1:F:298:ASP:OD1	2.34	0.49
3:K:800:PRO:HA	3:K:803:VAL:HG22	1.92	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
1:E:387:ILE:O	1:E:393:GLY:HA3	2.12	0.49
1:E:298:ASP:OD1	1:E:298:ASP:N	2.35	0.49
3:K:173:GLN:O	3:K:176:ILE:HD13	2.12	0.49
3:L:374:ALA:CB	3:L:398:GLU:OE2	2.59	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:459:ARG:NE	3:K:460:ASP:OD1	2.44	0.49
2:H:867:LEU:HD23	2:H:920:ILE:HG22	1.95	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
1:E:350:ILE:HD11	1:E:422:TYR:CE2	2.47	0.49
3:L:397:ALA:HB1	3:L:421:GLU:HG3	1.93	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:D:434:GLU:OE1	3:D:435:GLY:HA3	2.13	0.49
2:G:867:LEU:HD13	2:G:908:MET:HE1	1.94	0.49
2:B:796:VAL:HG13	2:B:838:LEU:HD21	1.95	0.49
2:G:826:THR:HG22	2:G:862:GLN:OE1	2.12	0.49
1:C:163:VAL:HG12	1:C:280:ILE:HD11	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:L:388:SER:HB3	3:L:389:HIS:CD2	2.48	0.49
3:K:519:THR:HG23	3:K:522:MET:CE	2.43	0.49
3:K:441:GLN:O	3:K:445:ILE:HG12	2.13	0.49
1:C:154:PRO:HG2	1:C:157:TYR:CE1	2.48	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
3:K:376:ILE:O	3:K:379:LEU:HB2	2.13	0.49
2:H:940:PRO:HA	2:H:942:ASN:N	2.28	0.49
1:E:191:PHE:HZ	1:E:309:TYR:CD2	2.30	0.49
3:J:177:TYR:CD2	3:J:363:TYR:CE1	3.00	0.49
2:H:796:VAL:HG13	2:H:838:LEU:HD21	1.94	0.49
2:H:981:LYS:HA	2:H:981:LYS:HE2	1.95	0.49
3:K:177:TYR:CD2	3:K:363:TYR:CE1	3.01	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
3:L:410:PHE:CD2	3:L:410:PHE:O	2.66	0.48
2:G:835:TYR:N	2:G:835:TYR:CD1	2.81	0.48
3:L:444:LYS:HE3	3:L:448:GLU:OE2	2.13	0.48
1:F:191:PHE:CZ	1:F:309:TYR:CD2	2.92	0.48
1:E:193:GLY:O	1:E:195:LEU:HG	2.13	0.48
1:C:151:PHE:HD1	1:C:152:LEU:N	2.10	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:380:LEU:HA	1:C:380:LEU:HD23	1.66	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
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:D:422:PHE:HB3	3:D:425:LEU:CD2	2.43	0.48
1:C:354:PHE:O	1:C:355:LYS:HG2	2.14	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
3:D:428:LEU:HB3	3:D:455:ILE:CD1	2.41	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:K:410:PHE:CG	3:K:410:PHE:O	2.66	0.48
1:C:219:PHE:HE1	3:K:356:TYR:CE1	2.32	0.48
1:F:348:TYR:CE1	1:F:376:LEU:HD13	2.49	0.48
1:F:151:PHE:HD1	1:F:152:LEU:N	2.12	0.48
3:K:804:SER:O	3:K:805:LYS:HB2	2.14	0.48
3:J:142:HIS:ND1	3:J:434:GLU:OE2	2.46	0.48
2:B:981:LYS:HE2	2:B:981:LYS:HA	1.96	0.48
3:J:347:PHE:CD1	3:J:368:SER:HB2	2.45	0.48
2:I:971:VAL:O	2:I:974:LYS:HB3	2.13	0.48
1:F:168:LEU:HD13	1:F:280:ILE:HD12	1.95	0.48
1:A:191:PHE:HD1	1:A:191:PHE:H	1.62	0.48
3:K:769:THR:O	3:K:818:HIS:HA	2.14	0.48
1:A:151:PHE:C	1:A:151:PHE:HD1	2.18	0.48
1:E:151:PHE:HD1	1:E:151:PHE:C	2.16	0.48
2:B:909:LEU:HD12	2:B:951:LEU:HD23	1.96	0.48
1:A:304:THR:HB	1:A:307:ALA:HB2	1.95	0.48
2:B:978:LEU:HB3	2:B:982:SER:OG	2.14	0.48
3:K:425:LEU:O	3:K:455:ILE:HD13	2.14	0.47
3:K:410:PHE:HE1	3:K:431:LEU:HD11	1.78	0.47
1:C:304:THR:HB	1:C:307:ALA:HB2	1.95	0.47
3:J:422:PHE:HB2	3:J:425:LEU:CG	2.40	0.47
3:D:425:LEU:O	3:D:455:ILE:HD13	2.14	0.47
1:A:354:PHE:O	1:A:355:LYS:CB	2.61	0.47
1:A:163:VAL:HG12	1:A:280:ILE:HD11	1.96	0.47
2:G:981:LYS:HE2	2:G:981:LYS:HA	1.96	0.47
1:A:194:THR:HG23	1:A:194:THR:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:397:ALA:C	3:K:399:LEU:N	2.65	0.47
2:G:971:VAL:O	2:G:974:LYS:HB3	2.13	0.47
1:F:258:SER:O	1:F:259:THR:C	2.53	0.47
2:H:791:PHE:HE1	2:H:795:ASN:ND2	2.12	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
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
1:C:247:ASN:HB3	1:C:275:HIS:CE1	2.49	0.47
1:C:273:GLU:OE1	1:C:273:GLU:N	2.47	0.47
3:D:441:GLN:O	3:D:445:ILE:HG12	2.15	0.47
3:K:423:GLY:C	3:K:425:LEU:N	2.67	0.47
3:D:346:ILE:O	3:D:369:LEU:HD12	2.15	0.47
1:F:344:LEU:HD21	1:F:376:LEU:HD23	1.95	0.47
3:L:372:LEU:HD12	3:L:373:PRO:HD2	1.95	0.47
1:F:346:LEU:HD23	1:F:346:LEU:O	2.13	0.47
1:F:182:TYR:CZ	1:F:237:PRO:HD3	2.50	0.47
2:I:901:LYS:HG2	2:I:902:ASN:N	2.29	0.47
3:D:451:VAL:O	3:D:454:LEU:N	2.47	0.47
3:K:536:ARG:O	3:K:540:LEU:HG	2.15	0.47
3:K:186:TYR:C	3:K:186:TYR:CD1	2.88	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:J:413:ASN:O	3:J:436:ASN:HB3	2.14	0.47
2:H:764:LEU:HD12	2:H:864:PHE:CD1	2.50	0.47
3:J:397:ALA:C	3:J:399:LEU:N	2.66	0.47
3:J:422:PHE:CB	3:J:425:LEU:CG	2.83	0.47
3:J:410:PHE:CZ	3:J:433:VAL:HG12	2.48	0.47
3:L:410:PHE:O	3:L:410:PHE:CG	2.68	0.47
3:K:143:PRO:HG3	3:K:443:LEU:HD13	1.97	0.47
1:C:193:GLY:C	1:C:195:LEU:HD23	2.35	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:D:769:THR:O	3:D:818:HIS:HA	2.14	0.47
2:H:834:ASN:HB2	2:H:835:TYR:CE1	2.49	0.47
2:G:809:LYS:HG3	2:G:846:MET:SD	2.55	0.47
1:E:182:TYR:CZ	1:E:237:PRO:HD3	2.50	0.47
2:I:788:LYS:O	2:I:792:VAL:HG23	2.14	0.47
1:F:225:LEU:HD23	1:F:225:LEU:C	2.35	0.47
3:L:413:ASN:O	3:L:436:ASN:HB3	2.14	0.47
3:D:579:PHE:HZ	3:D:598:GLY:HA3	1.79	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
1:C:179:VAL:HG23	1:C:294:LEU:HD23	1.97	0.47
1:A:191:PHE:HZ	1:A:309:TYR:CD2	2.32	0.47
2:G:796:VAL:HG13	2:G:838:LEU:HD21	1.97	0.47
3:K:244:LYS:CB	3:K:247:LEU:HB2	2.45	0.47
2:B:940:PRO:HA	2:B:942:ASN:N	2.29	0.47
1:A:154:PRO:HG2	1:A:157:TYR:CE1	2.50	0.47
3:K:152:LEU:H	3:K:152:LEU:HD12	1.79	0.47
3:D:173:GLN:CB	3:D:179:ARG:HH12	2.28	0.47
3:L:438:LEU:HD13	3:L:443:LEU:HD23	1.97	0.47
1:A:202:PHE:HB2	1:A:203:ARG:H	1.48	0.47
2:I:940:PRO:HA	2:I:942:ASN:H	1.79	0.47
3:D:177:TYR:CD2	3:D:363:TYR:CE1	3.03	0.47
3:K:163:LEU:HD11	3:K:249:GLU:CA	2.40	0.46
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:D:339:LEU:HB2	3:D:359:LEU:HD11	1.97	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
3:J:341:LEU:O	3:J:344:LEU:HD11	2.15	0.46
1:F:346:LEU:C	1:F:346:LEU:HD23	2.36	0.46
3:D:151:LEU:HB3	3:D:157:TRP:HB3	1.97	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:K:446:LEU:HA	3:K:450:SER:O	2.16	0.46
1:A:219:PHE:CD2	3:D:353:ILE:HG22	2.51	0.46
3:D:186:TYR:C	3:D:186:TYR:CD1	2.88	0.46
3:D:550:ASP:O	3:D:603:PHE:HA	2.16	0.46
3:J:422:PHE:C	3:J:422:PHE:CD1	2.88	0.46
3:D:384:VAL:HA	3:D:407:TYR:O	2.15	0.46
2:I:956:ASN:ND2	2:I:966:THR:HG23	2.29	0.46
2:H:956:ASN:OD1	2:H:966:THR:HG23	2.16	0.46
3:J:364:LEU:HA	3:J:364:LEU:HD23	1.76	0.46
3:K:372:LEU:HB3	3:K:396:PRO:HG3	1.97	0.46
1:A:219:PHE:CE1	3:D:353:ILE:HA	2.51	0.46
1:E:344:LEU:HD13	1:E:402:PHE:HB2	1.97	0.46
3:D:465:ILE:HA	3:D:466:PRO:HD2	1.68	0.46
2:H:880:LEU:CD2	2:H:920:ILE:HG23	2.45	0.46
2:H:812:LEU:HD23	2:H:846:MET:HE1	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:142:HIS:ND1	3:L:434:GLU:OE2	2.48	0.46
3:J:161:LEU:HD23	3:J:434:GLU:HG3	1.98	0.46
1:C:391:THR:O	1:C:394:GLN:HB2	2.16	0.46
2:G:978:LEU:HB3	2:G:982:SER:OG	2.15	0.46
1:A:380:LEU:HD23	1:A:380:LEU:HA	1.69	0.46
3:K:151:LEU:HB3	3:K:157:TRP:HB3	1.98	0.46
3:D:434:GLU:HA	3:D:435:GLY:HA2	1.54	0.46
1:A:252:PRO:HB3	1:A:257:MET:CE	2.45	0.46
2:I:835:TYR:CD1	2:I:835:TYR:N	2.83	0.46
3:K:431:LEU:O	3:K:431:LEU:HG	2.16	0.46
3:K:346:ILE:HD12	3:K:367:ASN:ND2	2.30	0.46
2:B:835:TYR:N	2:B:835:TYR:CD1	2.84	0.46
2:I:764:LEU:HD12	2:I:864:PHE:CD1	2.51	0.46
2:G:940:PRO:HA	2:G:942:ASN:H	1.81	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
2:B:764:LEU:HD12	2:B:864:PHE:CD1	2.51	0.46
3:K:397:ALA:HA	3:K:421:GLU:HG3	1.98	0.46
3:D:383:ARG:HA	3:D:405:LEU:HA	1.97	0.46
3:J:138:ASN:HB3	3:J:141:LEU:HD23	1.97	0.46
1:F:184:HIS:O	1:F:229:LEU:HA	2.16	0.46
3:D:143:PRO:HG3	3:D:443:LEU:HD13	1.98	0.45
3:L:422:PHE:C	3:L:422:PHE:CD1	2.89	0.45
3:K:356:TYR:CD2	3:K:358:PHE:HE1	2.33	0.45
2:I:834:ASN:HB2	2:I:835:TYR:CE1	2.51	0.45
2:B:834:ASN:HB2	2:B:835:TYR:CE1	2.51	0.45
2:B:788:LYS:O	2:B:792:VAL:HG23	2.16	0.45
3:J:379:LEU:HD23	3:J:379:LEU:HA	1.74	0.45
3:D:372:LEU:HB3	3:D:396:PRO:HG3	1.98	0.45
1:E:344:LEU:HD21	1:E:376:LEU:HD23	1.97	0.45
1:A:344:LEU:HD13	1:A:402:PHE:HB2	1.97	0.45
3:L:376:ILE:O	3:L:379:LEU:HB2	2.16	0.45
1:E:193:GLY:C	1:E:195:LEU:CD2	2.85	0.45
3:K:434:GLU:HA	3:K:435:GLY:HA2	1.55	0.45
1:C:380:LEU:HD22	1:C:404:GLN:HG2	1.98	0.45
1:E:219:PHE:CZ	3:L:356:TYR:CE2	3.04	0.45
2:H:911:GLU:O	2:H:915:GLU:HG2	2.15	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:J:372:LEU:HA	3:J:373:PRO:HD2	1.87	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: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
1:C:165:LYS:NZ	1:C:165:LYS:HB3	2.30	0.45
3:K:396:PRO:C	3:K:397:ALA:O	2.53	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:978:LEU:HB3	2:H:982:SER:OG	2.17	0.45
2:H:921:VAL:O	2:H:924:PHE:HB3	2.17	0.45
3:L:420:TRP:NE1	3:L:463:PRO:CD	2.80	0.45
3:K:452:THR:HA	3:K:455:ILE:HB	1.99	0.45
1:F:402:PHE:C	1:F:402:PHE:CD1	2.90	0.45
3:D:579:PHE:O	3:D:579:PHE:CD1	2.70	0.45
2:G:951:LEU:HD13	2:G:988:PHE:HD2	1.82	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
1:C:168:LEU:HD13	1:C:280:ILE:HD12	1.99	0.45
1:A:154:PRO:HG2	1:A:157:TYR:CD1	2.51	0.45
2:I:791:PHE:HE1	2:I:795:ASN:ND2	2.14	0.45
2:G:813:THR:HG22	2:G:814:PRO:HD2	1.99	0.45
3:J:375:GLU:C	3:J:377:LYS:N	2.69	0.45
1:A:201:THR:O	1:A:202:PHE:CD2	2.70	0.45
3:K:766:LEU:HD12	3:K:766:LEU:HA	1.73	0.45
1:C:354:PHE:CE2	1:C:415:ASN:ND2	2.85	0.45
2:I:796:VAL:HG13	2:I:838:LEU:HD21	1.99	0.45
2:H:835:TYR:N	2:H:835:TYR:CD1	2.84	0.45
2:H:929:LEU:HD23	2:H:929:LEU:HA	1.61	0.45
3:K:384:VAL:HA	3:K:407:TYR:O	2.16	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
1:A:179:VAL:HG23	1:A:294:LEU:HD23	1.99	0.45
3:J:342:SER:HA	3:J:365:ASN:O	2.17	0.45
1:C:348:TYR:CE1	1:C:376:LEU:HD13	2.52	0.45
3:L:345:GLN:CD	3:L:345:GLN:H	2.19	0.45
2:B:812:LEU:HD23	2:B:846:MET:HE1	1.99	0.45
2:G:812:LEU:HD23	2:G:846:MET:CE	2.47	0.45
1:E:263:GLU:OE1	1:E:263:GLU:HA	2.16	0.45
2:G:907:GLU:N	2:G:907:GLU:OE1	2.35	0.45
1:E:258:SER:O	1:E:259:THR:C	2.55	0.45
3:D:431:LEU:HG	3:D:431:LEU:O	2.17	0.45
1:C:202:PHE:O	1:C:203:ARG:HG3	2.17	0.45
3:L:180:GLN:OE1	3:L:244:LYS:HA	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:249:GLU:HA	1:F:275:HIS:O	2.16	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
3:D:424:ASN:ND2	3:D:807:ILE:CG2	2.73	0.44
3:L:379:LEU:HA	3:L:379:LEU:HD23	1.77	0.44
3:J:415:VAL:H	3:J:436:ASN:CB	2.30	0.44
2:B:837:ASP:O	2:B:840:SER:HB3	2.17	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
3:J:387:LEU:HD13	3:J:392:LEU:HD11	1.98	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:C:301:THR:HG23	1:C:340:ASN:OD1	2.17	0.44
3:L:462:ARG:HA	3:L:463:PRO:HD3	1.67	0.44
1:A:256:ILE:HG12	3:D:349:ILE:HA	2.00	0.44
1:C:191:PHE:HZ	1:C:309:TYR:CD2	2.35	0.44
3:L:361:ARG:O	3:L:384:VAL:O	2.35	0.44
3:K:383:ARG:HA	3:K:405:LEU:HA	1.98	0.44
3:J:361:ARG:O	3:J:384:VAL:O	2.35	0.44
1:C:168:LEU:HD22	1:C:280:ILE:HG23	1.99	0.44
2:I:929:LEU:HA	2:I:929:LEU:HD23	1.59	0.44
1:F:391:THR:O	1:F:394:GLN:HB2	2.18	0.44
1:C:258:SER:O	1:C:260:GLU:N	2.50	0.44
3:K:339:LEU:HB2	3:K:359:LEU:HD11	2.00	0.44
3:J:418:LEU:CD1	3:J:454:LEU:HD21	2.47	0.44
3:J:176:ILE:HD11	3:J:343:ASN:ND2	2.32	0.44
1:F:199:ILE:HG22	1:F:200:GLY:N	2.32	0.44
1:A:249:GLU:HA	1:A:275:HIS:O	2.18	0.44
3:J:392:LEU:O	3:J:413:ASN:HB3	2.18	0.44
1:A:380:LEU:HD22	1:A:404:GLN:HG2	2.00	0.44
2:G:901:LYS:HG2	2:G:902:ASN:N	2.33	0.44
3:L:375:GLU:CD	3:L:375:GLU:H	2.20	0.44
3:L:363:TYR:HE1	3:L:384:VAL:HG11	1.82	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: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
3:D:810:PRO:HB3	3:D:816:SER:N	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:445:ILE:CD1	3:J:457:TYR:CD2	3.01	0.44
3:D:514:CYS:HG	3:D:517:TYR:HD1	1.66	0.44
3:D:441:GLN:HA	3:D:444:LYS:HD2	2.00	0.44
2:I:812:LEU:HD23	2:I:846:MET:CE	2.48	0.44
3:K:544:ILE:HG23	3:K:552:LEU:CD1	2.47	0.44
3:J:394:SER:O	3:J:395:LEU:HD23	2.17	0.44
3:D:555:GLN:C	3:D:599:CYS:SG	2.96	0.44
1:C:336:GLN:HB3	2:H:937:ILE:HD11	1.99	0.44
2:B:929:LEU:HA	2:B:929:LEU:HD23	1.65	0.44
3:D:768:PHE:HA	3:D:778:VAL:HG22	2.00	0.43
3:L:388:SER:CB	3:L:389:HIS:CD2	3.01	0.43
3:K:177:TYR:HE1	3:K:365:ASN:HD21	1.65	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:450:SER:OG	3:K:451:VAL:N	2.50	0.43
1:A:193:GLY:O	1:A:195:LEU:HG	2.18	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
2:I:809:LYS:HG3	2:I:846:MET:SD	2.58	0.43
1:F:185:VAL:HG23	1:F:229:LEU:HD12	2.00	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
3:K:420:TRP:C	3:K:422:PHE:O	2.57	0.43
3:D:392:LEU:CB	3:D:413:ASN:HD22	2.23	0.43
3:D:160:GLN:NE2	3:D:430:PHE:CZ	2.85	0.43
3:D:152:LEU:HD12	3:D:152:LEU:N	2.33	0.43
3:K:551:LEU:HD21	3:K:601:ILE:HG23	2.00	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:D:441:GLN:O	3:D:444:LYS:HB2	2.18	0.43
3:K:441:GLN:HA	3:K:444:LYS:HD2	2.00	0.43
3:K:436:ASN:N	3:K:436:ASN:OD1	2.52	0.43
3:J:343:ASN:OD1	3:J:366:GLY:HA3	2.17	0.43
2:H:880:LEU:HD22	2:H:920:ILE:HG23	1.99	0.43
1:C:199:ILE:HG22	1:C:200:GLY:N	2.32	0.43
3:D:544:ILE:HG23	3:D:552:LEU:CD1	2.48	0.43
3:L:375:GLU:OE1	3:L:375:GLU:N	2.52	0.43
3:D:389:HIS:HA	3:D:412:ASP:HB3	2.00	0.43
1:C:386:SER:O	1:C:389:THR:HG23	2.18	0.43
3:D:766:LEU:HA	3:D:766:LEU:HD12	1.74	0.43
3:D:356:TYR:CD2	3:D:358:PHE:HE1	2.36	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:369:LEU:HD12	3:D:369:LEU:N	2.33	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
3:J:341:LEU:O	3:J:344:LEU:CD1	2.67	0.43
3:K:254:LEU:HA	3:K:254:LEU:HD23	1.70	0.43
2:G:929:LEU:HD23	2:G:929:LEU:HA	1.55	0.43
1:E:332:TRP:CZ2	1:E:336:GLN:HG3	2.54	0.43
1:A:165:LYS:NZ	1:A:165:LYS:HB3	2.33	0.43
3:K:445:ILE:HG13	3:K:457:TYR:HD2	1.84	0.43
3:D:163:LEU:HD23	3:D:163:LEU:HA	1.78	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
1:E:346:LEU:O	1:E:346:LEU:HD23	2.18	0.43
2:I:813:THR:HG22	2:I:814:PRO:CD	2.49	0.43
1:C:249:GLU:HA	1:C:275:HIS:O	2.19	0.43
3:L:394:SER:O	3:L:395:LEU:HD23	2.18	0.43
3:J:410:PHE:HE1	3:J:431:LEU:HD11	1.84	0.43
3:L:418:LEU:HB3	3:L:422:PHE:CE1	2.53	0.43
3:K:392:LEU:CB	3:K:413:ASN:HD22	2.24	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:L:387:LEU:HD13	3:L:392:LEU:HD11	2.00	0.43
1:E:289:LEU:HD23	1:E:318:LEU:HD21	2.01	0.43
1:E:247:ASN:HB3	1:E:275:HIS:CE1	2.53	0.43
3:K:371:GLU:HG2	3:K:372:LEU:N	2.33	0.43
3:J:356:TYR:HB3	3:J:358:PHE:HE1	1.83	0.43
3:D:769:THR:CG2	3:D:778:VAL:HG13	2.49	0.43
2:H:956:ASN:OD1	2:H:966:THR:HA	2.19	0.43
2:G:880:LEU:CD2	2:G:920:ILE:HG23	2.49	0.43
3:L:457:TYR:HE1	3:L:461:ASN:ND2	2.17	0.43
1:C:179:VAL:CG2	1:C:294:LEU:HD23	2.49	0.43
3:J:422:PHE:HA	3:J:424:ASN:H	1.80	0.43
3:D:396:PRO:C	3:D:397:ALA:O	2.56	0.43
3:L:415:VAL:H	3:L:436:ASN:CB	2.32	0.43
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
3:J:415:VAL:H	3:J:436:ASN:HB3	1.84	0.42
2:I:940:PRO:HA	2:I:942:ASN:N	2.34	0.42
1:C:227:LEU:HA	1:C:227:LEU:HD23	1.82	0.42
3:J:408:PHE:C	3:J:408:PHE:CD1	2.91	0.42
3:D:173:GLN:O	3:D:176:ILE:CD1	2.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:956:ASN:OD1	2:I:966:THR:HA	2.19	0.42
2:G:956:ASN:OD1	2:G:966:THR:HA	2.20	0.42
1:F:182:TYR:CE2	1:F:237:PRO:HD3	2.54	0.42
1:A:325:ASN:HB2	1:A:326:ASN:HD22	1.84	0.42
1:F:380:LEU:HD22	1:F:404:GLN:HG2	2.00	0.42
2:I:921:VAL:O	2:I:924:PHE:HB3	2.19	0.42
1:F:263:GLU:HA	1:F:263:GLU:OE1	2.19	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
3:K:413:ASN:HB2	3:K:436:ASN:ND2	2.34	0.42
3:K:354:PHE:HE2	3:K:373:PRO:HG2	1.81	0.42
3:D:150:SER:HA	3:D:152:LEU:CD1	2.50	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: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:809:PHE:HB3	3:K:810:PRO:HA	2.01	0.42
1:E:387:ILE:O	1:E:390:THR:HG23	2.18	0.42
3:K:365:ASN:N	3:K:365:ASN:OD1	2.49	0.42
3:D:365:ASN:N	3:D:365:ASN:OD1	2.49	0.42
1:A:336:GLN:HB3	2:B:937:ILE:HD11	2.00	0.42
1:A:158:LEU:HD11	1:A:385:PHE:CE2	2.54	0.42
2:G:764:LEU:HD12	2:G:864:PHE:CD1	2.55	0.42
3:D:812:ASP:C	3:D:812:ASP:OD1	2.58	0.42
3:J:383:ARG:HG2	3:J:406:LYS:HG3	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:D:445:ILE:HG13	3:D:457:TYR:HD2	1.84	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
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
2:B:813:THR:HG22	2:B:814:PRO:CD	2.50	0.42
3:L:445:ILE:CD1	3:L:457:TYR:CD2	3.02	0.42
2:I:929:LEU:HB3	2:I:972:LEU:HD11	2.00	0.42
1:C:325:ASN:HB2	1:C:326:ASN:HD22	1.84	0.42
1:C:265:LEU:O	1:C:268:SER:HB3	2.20	0.42
3:K:812:ASP:OD1	3:K:812:ASP:C	2.58	0.42
1:F:332:TRP:CZ2	1:F:336:GLN:HG3	2.55	0.42
3:D:170:SER:O	3:D:176:ILE:HD12	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:374:ALA:C	3:D:376:ILE:N	2.73	0.42
1:F:202:PHE:HB2	1:F:203:ARG:H	1.45	0.42
1:E:202:PHE:CZ	1:E:208:TYR:HD1	2.38	0.42
1:C:354:PHE:O	1:C:355:LYS:CB	2.67	0.42
3:D:536:ARG:O	3:D:540:LEU:HG	2.20	0.42
1:E:346:LEU:HD23	1:E:346:LEU:C	2.40	0.42
1:E:219:PHE:HZ	3:L:356:TYR:CE2	2.37	0.42
3:K:551:LEU:HD21	3:K:601:ILE:CG2	2.50	0.42
3:J:464:GLU:HB3	3:J:465:ILE:H	1.57	0.42
3:L:423:GLY:H	3:L:458:LEU:HB2	1.85	0.42
3:K:459:ARG:HD3	3:K:524:ARG:O	2.20	0.42
3:K:163:LEU:HA	3:K:163:LEU:HD23	1.79	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:L:418:LEU:CD1	3:L:454:LEU:HD21	2.49	0.42
3:D:353:ILE:O	3:D:356:TYR:HB2	2.19	0.42
1:A:193:GLY:C	1:A:195:LEU:HD23	2.40	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:867:LEU:HD13	2:H:908:MET:HE1	2.02	0.42
2:H:813:THR:HB	2:H:815:ASN:OD1	2.20	0.42
1:E:184:HIS:O	1:E:229:LEU:HA	2.20	0.42
3:D:157:TRP:CZ3	3:D:443:LEU:HD22	2.48	0.42
1:C:354:PHE:CZ	1:C:415:ASN:ND2	2.88	0.42
2:H:837:ASP:O	2:H:840:SER:HB3	2.20	0.42
3:L:349:ILE:HA	3:L:349:ILE:HD13	1.87	0.42
3:J:369:LEU:N	3:J:390:ASN:OD1	2.52	0.42
3:K:170:SER:O	3:K:176:ILE:HD12	2.20	0.41
3:L:420:TRP:CD1	3:L:463:PRO:HD2	2.55	0.41
3:L:176:ILE:HG13	3:L:176:ILE:H	1.39	0.41
1:C:354:PHE:HE2	1:C:415:ASN:HB3	1.85	0.41
3:K:405:LEU:HD13	3:K:408:PHE:HB2	2.01	0.41
3:J:141:LEU:HD11	3:J:437:PRO:HD3	2.01	0.41
1:C:350:ILE:CD1	1:C:422:TYR:CZ	3.03	0.41
2:H:792:VAL:HG11	2:H:808:LEU:HB2	2.02	0.41
2:G:940:PRO:HA	2:G:942:ASN:N	2.35	0.41
3:J:375:GLU:H	3:J:375:GLU:CD	2.22	0.41
3:D:514:CYS:SG	3:D:517:TYR:HD1	2.43	0.41
3:L:364:LEU:HA	3:L:364:LEU:HD23	1.83	0.41
3:K:513:LEU:HB3	3:K:536:ARG:NH2	2.35	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)
1:A:422:TYR:CD1	1:A:422:TYR:N	2.88	0.41
1:E:199:ILE:HG22	1:E:200:GLY:N	2.34	0.41
3:K:177:TYR:OH	3:K:386:ASP:OD2	2.39	0.41
1:F:380:LEU:HA	1:F:380:LEU:HD23	1.71	0.41
3:J:464:GLU:O	3:J:465:ILE:CB	2.67	0.41
3:D:166:VAL:HG21	3:D:248:MET:HG3	2.02	0.41
3:L:245:GLN:NE2	3:L:409:TYR:CE2	2.88	0.41
1:E:165:LYS:HB3	1:E:165:LYS:NZ	2.36	0.41
3:L:343:ASN:OD1	3:L:366:GLY:HA3	2.19	0.41
3:J:150:SER:CA	3:J:152:LEU:HD12	2.34	0.41
1:A:219:PHE:CE1	3:D:356:TYR:CE1	3.08	0.41
3:L:372:LEU:HA	3:L:373:PRO:HD2	1.82	0.41
1:F:193:GLY:O	1:F:195:LEU:HG	2.20	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
2:G:977:ASN:O	2:G:978:LEU:HD23	2.20	0.41
3:L:408:PHE:CD1	3:L:408:PHE:C	2.92	0.41
3:J:422:PHE:CA	3:J:424:ASN:H	2.33	0.41
3:J:420:TRP:O	3:J:422:PHE:O	2.38	0.41
3:D:379:LEU:HA	3:D:379:LEU:HD23	1.82	0.41
3:K:353:ILE:O	3:K:356:TYR:HB2	2.20	0.41
3:D:346:ILE:HD12	3:D:367:ASN:ND2	2.35	0.41
1:A:256:ILE:HG13	3:D:350:SER:H	1.85	0.41
3:L:379:LEU:HB3	3:L:382:LEU:HD13	2.03	0.41
3:L:180:GLN:OE1	3:L:244:LYS:N	2.54	0.41
3:K:810:PRO:HB3	3:K:816:SER:N	2.35	0.41
2:I:909:LEU:HD12	2:I:951:LEU:HD23	2.03	0.41
1:A:354:PHE:CE2	1:A:415:ASN:ND2	2.89	0.41
2:H:909:LEU:HD21	2:H:925:VAL:HG21	2.02	0.41
2:G:812:LEU:HD23	2:G:846:MET:HE2	2.02	0.41
3:J:444:LYS:O	3:J:447:THR:O	2.38	0.41
3:L:392:LEU:O	3:L:413:ASN:HB3	2.21	0.41
2:G:803:ASN:O	2:G:806:ASP:N	2.53	0.41
1:E:325:ASN:HB2	1:E:326:ASN:HD22	1.85	0.41
2:B:827:GLN:HA	2:B:827:GLN:OE1	2.21	0.41
3:D:400:GLY:O	3:D:424:ASN:ND2	2.52	0.41
3:L:419:PRO:HG2	3:L:422:PHE:CE1	2.55	0.41
1:A:256:ILE:CG1	3:D:350:SER:H	2.34	0.41
3:K:768:PHE:HA	3:K:778:VAL:HG22	2.03	0.41
2:G:956:ASN:ND2	2:G:966:THR:HG23	2.33	0.41
1:C:387:ILE:O	1:C:390:THR:HG23	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:380:LEU:HD23	1:E:380:LEU:HA	1.71	0.41
1:C:289:LEU:HD23	1:C:318:LEU:HD21	2.01	0.41
1:E:343:ASP:OD1	1:E:345:ASN:HB3	2.21	0.41
3:J:349:ILE:HA	3:J:349:ILE:HD13	1.90	0.41
3:L:419:PRO:CD	3:L:422:PHE:HE1	2.33	0.41
1:A:426:ILE:HG22	1:A:427:TYR:N	2.23	0.41
3:D:768:PHE:CD1	3:D:768:PHE:N	2.89	0.41
1:A:199:ILE:HG22	1:A:200:GLY:N	2.35	0.41
2:H:820:PHE:CD1	2:H:820:PHE:C	2.92	0.41
2:I:910:ILE:HG22	2:I:914:LYS:HE2	2.02	0.41
3:D:522:MET:C	3:D:523:TYR:CD1	2.94	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
2:H:979:THR:C	2:H:981:LYS:N	2.74	0.41
1:F:258:SER:C	1:F:260:GLU:N	2.73	0.41
2:H:791:PHE:CE1	2:H:795:ASN:ND2	2.89	0.41
2:H:929:LEU:HB3	2:H:972:LEU:HD11	2.02	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
1:F:314:LEU:HA	1:F:314:LEU:HD12	1.78	0.41
1:C:287:GLN:HG2	2:H:944:TRP:HA	2.02	0.41
3:K:440:LYS:HA	3:K:443:LEU:HB2	2.03	0.41
3:D:163:LEU:HD11	3:D:249:GLU:CA	2.41	0.41
3:K:369:LEU:N	3:K:369:LEU:HD12	2.36	0.41
2:I:909:LEU:HD21	2:I:925:VAL:HG21	2.02	0.41
2:G:936:LYS:HA	2:G:939:LYS:HE2	2.03	0.41
3:J:462:ARG:HA	3:J:463:PRO:HD3	1.70	0.41
3:L:420:TRP:CZ2	3:L:463:PRO:HD3	2.54	0.41
3:K:425:LEU:HD12	3:K:425:LEU:O	2.21	0.41
3:K:441:GLN:O	3:K:444:LYS:HB2	2.21	0.41
3:D:254:LEU:HD23	3:D:254:LEU:HA	1.74	0.41
3:L:163:LEU:HA	3:L:163:LEU:HD23	1.86	0.41
1:F:346:LEU:HD23	1:F:350:ILE:HG13	2.03	0.41
1:E:182:TYR:CE2	1:E:237:PRO:HD3	2.56	0.41
3:J:388:SER:CB	3:J:389:HIS:CD2	3.04	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
1:E:314:LEU:HA	1:E:314:LEU:HD12	1.78	0.41
1:A:184:HIS:O	1:A:229:LEU:HA	2.21	0.41
3:D:456:PHE:O	3:D:457:TYR:C	2.56	0.41
3:L:397:ALA:C	3:L:399:LEU:N	2.74	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:201:THR:C	1:C:202:PHE:CG	2.93	0.41
3:J:346:ILE:HD13	3:J:346:ILE:HG21	1.58	0.41
3:D:513:LEU:HB3	3:D:536:ARG:NH2	2.36	0.41
1:C:390:THR:HG1	1:C:393:GLY:H	1.64	0.41
1:A:311:LEU:HD21	1:A:338:MET:HE1	2.03	0.41
1:F:163:VAL:HG12	1:F:280:ILE:HD11	2.02	0.41
3:D:177:TYR:HE1	3:D:365:ASN:HD21	1.68	0.41
3:L:408:PHE:CD1	3:L:409:TYR:N	2.89	0.41
1:A:182:TYR:CE2	1:A:237:PRO:HD3	2.56	0.41
1:C:320:ASN:HB3	2:H:941:PRO:O	2.21	0.41
3:D:336:TRP:O	3:D:336:TRP:CG	2.72	0.41
2:B:911:GLU:O	2:B:915:GLU:HG2	2.20	0.41
2:G:762:ILE:HB	2:G:763:PRO:HD2	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: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
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
3:D:176:ILE:HG12	3:D:176:ILE:H	1.49	0.40
3:J:418:LEU:HB3	3:J:422:PHE:CE1	2.55	0.40
1:C:202:PHE:C	1:C:203:ARG:HG3	2.41	0.40
1:A:202:PHE:O	1:A:203:ARG:HG3	2.21	0.40
3:J:356:TYR:HB3	3:J:358:PHE:CE1	2.56	0.40
3:K:768:PHE:HA	3:K:777:ASP:O	2.21	0.40
3:K:563:GLU:H	3:K:563:GLU:HG2	1.77	0.40
1:E:350:ILE:CD1	1:E:422:TYR:CZ	3.04	0.40
1:A:258:SER:O	1:A:260:GLU:N	2.54	0.40
1:E:225:LEU:HD23	1:E:225:LEU:C	2.42	0.40
3:D:458:LEU:O	3:D:459:ARG:C	2.59	0.40
3:K:379:LEU:HA	3:K:379:LEU:HD23	1.78	0.40
1:E:402:PHE:C	1:E:402:PHE:CD1	2.94	0.40
3:L:403:PHE:C	3:L:403:PHE:CD1	2.95	0.40
3:J:411:PHE:O	3:J:412:ASP:HB3	2.21	0.40
2:G:791:PHE:CE1	2:G:795:ASN:ND2	2.90	0.40
1:A:168:LEU:HD22	1:A:280:ILE:HG23	2.03	0.40
3:D:177:TYR:OH	3:D:386:ASP:OD2	2.40	0.40
3:D:135:ASN:HA	3:D:138:ASN:HB2	2.04	0.40
1:A:225:LEU:C	1:A:225:LEU:HD23	2.41	0.40
3:J:410:PHE:CD2	3:J:410:PHE:O	2.75	0.40
3:L:420:TRP:O	3:L:422:PHE:O	2.39	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:942:ASN:OD1	2:H:944:TRP:HB3	2.21	0.40
1:E:305:TYR:O	1:E:306:HIS:HB3	2.20	0.40
3:D:465:ILE:HD13	3:D:465:ILE:HA	1.85	0.40
1:C:257:MET:O	3:K:347:PHE:CD1	2.74	0.40
3:J:177:TYR:CE2	3:J:363:TYR:CE1	3.10	0.40
3:L:414:MET:HA	3:L:437:PRO:HD2	2.03	0.40
3:D:522:MET:C	3:D:523:TYR:HD1	2.24	0.40
1:A:350:ILE:CD1	1:A:422:TYR:CZ	3.04	0.40
3:L:408:PHE:HD1	3:L:409:TYR:N	2.20	0.40
3:D:521:LYS:HA	3:D:524:ARG:NH1	2.37	0.40
3:K:173:GLN:O	3:K:176:ILE:CD1	2.70	0.40
1:E:405:LEU:HD12	1:E:405:LEU:O	2.21	0.40
3:L:341:LEU:O	3:L:344:LEU:HD11	2.21	0.40
1:E:354:PHE:CE2	1:E:415:ASN:ND2	2.90	0.40
1:E:346:LEU:HD23	1:E:350:ILE:HG13	2.04	0.40
1:F:346:LEU:O	1:F:350:ILE:HG13	2.22	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
3:K:420:TRP:O	3:K:422:PHE:N	2.54	0.40
1:E:202:PHE:CE1	3:L:336:TRP:CB	3.04	0.40
1:A:305:TYR:CD1	1:A:344:LEU:HD23	2.57	0.40
3:D:809:PHE:HB3	3:D:810:PRO:HA	2.03	0.40
3:K:768:PHE:CD1	3:K:768:PHE:N	2.90	0.40
3:J:457:TYR:HE1	3:J:461:ASN:ND2	2.19	0.40
2:H:861:ARG:O	2:H:864:PHE:HB3	2.21	0.40
1:F:185:VAL:HG23	1:F:229:LEU:CD1	2.51	0.40
1:C:258:SER:C	1:C:260:GLU:N	2.70	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

5.3.1 Protein backbone

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%)	39	79
1	C	263/288 (91%)	250 (95%)	12 (5%)	1 (0%)	39	79
1	E	263/288 (91%)	249 (95%)	13 (5%)	1 (0%)	39	79
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%)	46	83
3	J	204/727 (28%)	168 (82%)	34 (17%)	2 (1%)	19	64
3	K	300/727 (41%)	253 (84%)	46 (15%)	1 (0%)	46	83
3	L	204/727 (28%)	171 (84%)	31 (15%)	2 (1%)	19	64
All	All	2984/5056 (59%)	2731 (92%)	244 (8%)	9 (0%)	46	83

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 ⓘ

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%)	9	38
1	C	242/264 (92%)	218 (90%)	24 (10%)	10	41
1	E	242/264 (92%)	220 (91%)	22 (9%)	12	45
1	F	241/264 (91%)	218 (90%)	23 (10%)	11	43
2	B	211/231 (91%)	199 (94%)	12 (6%)	25	66
2	G	211/231 (91%)	198 (94%)	13 (6%)	23	63
2	H	211/231 (91%)	199 (94%)	12 (6%)	25	66
2	I	211/231 (91%)	198 (94%)	13 (6%)	23	63
3	D	258/648 (40%)	206 (80%)	52 (20%)	1	7
3	J	165/648 (26%)	129 (78%)	36 (22%)	1	6
3	K	261/648 (40%)	208 (80%)	53 (20%)	1	7
3	L	165/648 (26%)	130 (79%)	35 (21%)	1	6
All	All	2659/4572 (58%)	2339 (88%)	320 (12%)	6	30

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

Some 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 ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	267/288 (92%)	-0.16	2 (0%) 89 84	36, 58, 98, 121	0
1	C	267/288 (92%)	-0.16	3 (1%) 82 76	36, 58, 99, 121	0
1	E	267/288 (92%)	-0.23	0 100 100	35, 58, 100, 121	0
1	F	267/288 (92%)	-0.19	1 (0%) 93 91	36, 59, 98, 124	0
2	B	233/249 (93%)	0.02	6 (2%) 59 54	48, 79, 115, 146	0
2	G	233/249 (93%)	-0.08	3 (1%) 79 73	49, 81, 112, 146	0
2	H	233/249 (93%)	0.07	4 (1%) 73 67	48, 80, 115, 145	0
2	I	233/249 (93%)	-0.03	5 (2%) 67 62	50, 81, 114, 145	0
3	D	318/727 (43%)	0.14	16 (5%) 32 28	50, 87, 136, 160	0
3	J	210/727 (28%)	-0.28	5 (2%) 62 57	35, 61, 101, 127	0
3	K	318/727 (43%)	0.21	25 (7%) 15 15	50, 87, 136, 160	0
3	L	210/727 (28%)	-0.22	3 (1%) 78 72	35, 62, 102, 131	0
All	All	3056/5056 (60%)	-0.06	73 (2%) 62 57	35, 72, 115, 160	0

All (73) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	K	597	ASP	5.6
3	K	135	ASN	4.5
2	B	991	THR	4.4
3	L	466	PRO	4.0
2	H	991	THR	3.9
3	K	149	PRO	3.6
2	H	801	LEU	3.6
3	K	259	THR	3.6
1	C	355	LYS	3.5
3	K	517	TYR	3.5
3	D	259	THR	3.4

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Mol	Chain	Res	Type	RSRZ
2	I	961	TRP	3.3
3	D	135	ASN	3.3
1	A	371	TYR	3.3
3	K	551	LEU	3.3
3	K	598	GLY	3.3
3	D	257	SER	3.2
3	K	516	HIS	3.2
2	H	805	VAL	3.0
2	I	989	ILE	3.0
3	K	557	VAL	3.0
3	D	551	LEU	2.9
3	D	242	CYS	2.9
3	K	145	HIS	2.9
3	K	596	VAL	2.9
2	G	872	GLU	2.8
3	L	423	GLY	2.8
3	J	187	LEU	2.7
1	C	371	TYR	2.7
2	B	782	PRO	2.7
3	D	149	PRO	2.7
3	K	242	CYS	2.6
3	K	257	SER	2.6
3	K	778	VAL	2.6
3	K	562	PHE	2.6
3	K	134	VAL	2.6
2	I	872	GLU	2.6
3	K	766	LEU	2.5
2	G	870	LYS	2.5
3	D	137	SER	2.5
3	J	149	PRO	2.5
2	H	809	LYS	2.5
3	D	801	GLU	2.5
3	D	598	GLY	2.4
3	K	603	PHE	2.4
3	D	550	ASP	2.4
3	D	597	ASP	2.4
3	D	255	THR	2.4
3	K	137	SER	2.3
3	K	601	ILE	2.3
1	A	356	ASN	2.3
2	I	791	PHE	2.2
3	K	600	CYS	2.2

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Mol	Chain	Res	Type	RSRZ
3	D	562	PHE	2.2
3	J	153	ASN	2.2
1	C	259	THR	2.2
2	B	784	ASP	2.2
3	K	599	CYS	2.2
3	K	183	MET	2.1
3	K	554	LEU	2.1
3	J	186	TYR	2.1
1	F	414	PRO	2.1
3	K	518	ALA	2.1
2	B	809	LYS	2.1
3	J	252	ASP	2.0
2	B	839	TYR	2.0
3	D	601	ILE	2.0
3	D	800	PRO	2.0
3	D	769	THR	2.0
3	L	149	PRO	2.0
2	B	781	ALA	2.0
2	G	965	LEU	2.0
2	I	956	ASN	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.