



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 02:14 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 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/ValidationPDFNotes.html>

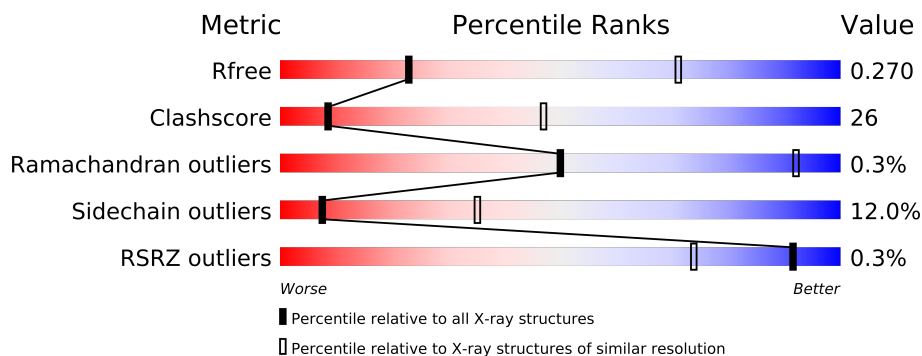
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

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}	66092	1013 (3.54-3.30)
Clashscore	79885	1270 (3.54-3.30)
Ramachandran outliers	78287	1232 (3.54-3.30)
Sidechain outliers	78261	1232 (3.54-3.30)
RSRZ outliers	66119	1013 (3.54-3.30)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	288	
1	C	288	
1	E	288	
1	F	288	
2	B	249	
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 hydrogen and 0 are deuterium.

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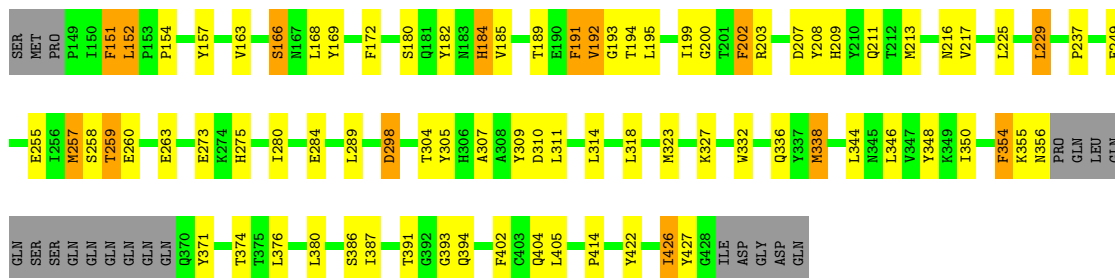
Chain	Residue	Modelled	Actual	Comment	Reference
H	754	MET	-	EXPRESSION TAG	UNP P25655
I	752	ARG	-	EXPRESSION TAG	UNP P25655
I	753	SER	-	EXPRESSION TAG	UNP P25655
I	754	MET	-	EXPRESSION TAG	UNP P25655

- 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			

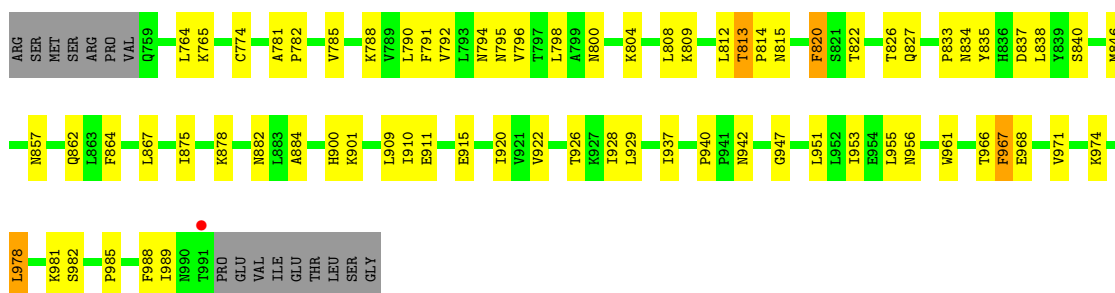
- Molecule 1: POLY(A) RIBONUCLEASE POP2

Chain F:



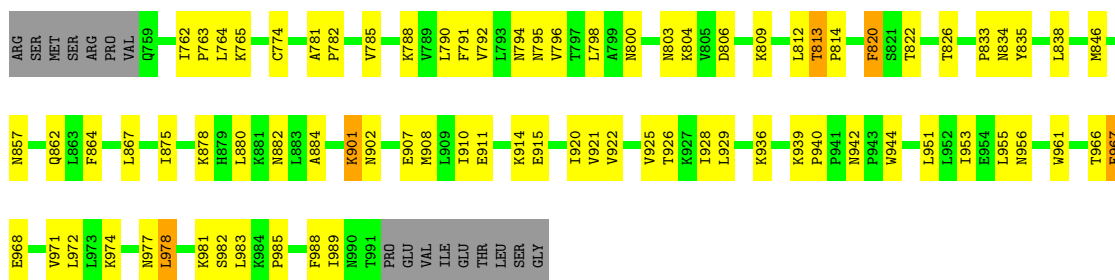
- Molecule 2: GENERAL NEGATIVE REGULATOR OF TRANSCRIPTION SUBUNIT 1

Chain B:



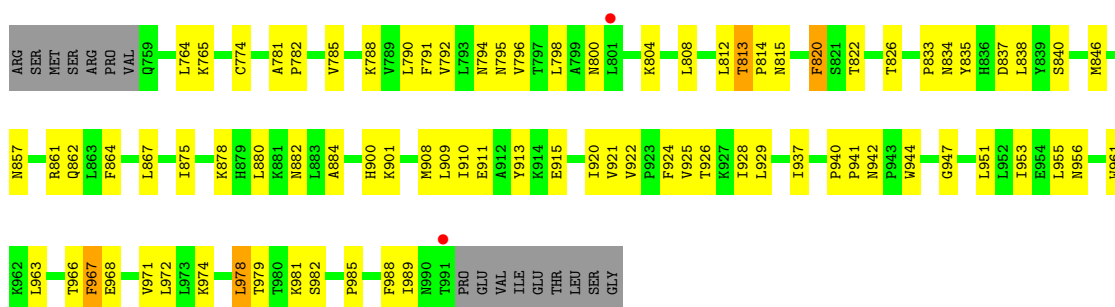
- Molecule 2: GENERAL NEGATIVE REGULATOR OF TRANSCRIPTION SUBUNIT 1

Chain G:



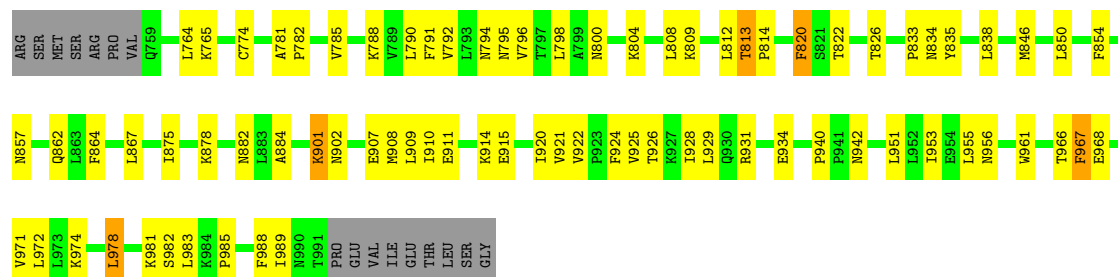
- Molecule 2: GENERAL NEGATIVE REGULATOR OF TRANSCRIPTION SUBUNIT 1

Chain H:



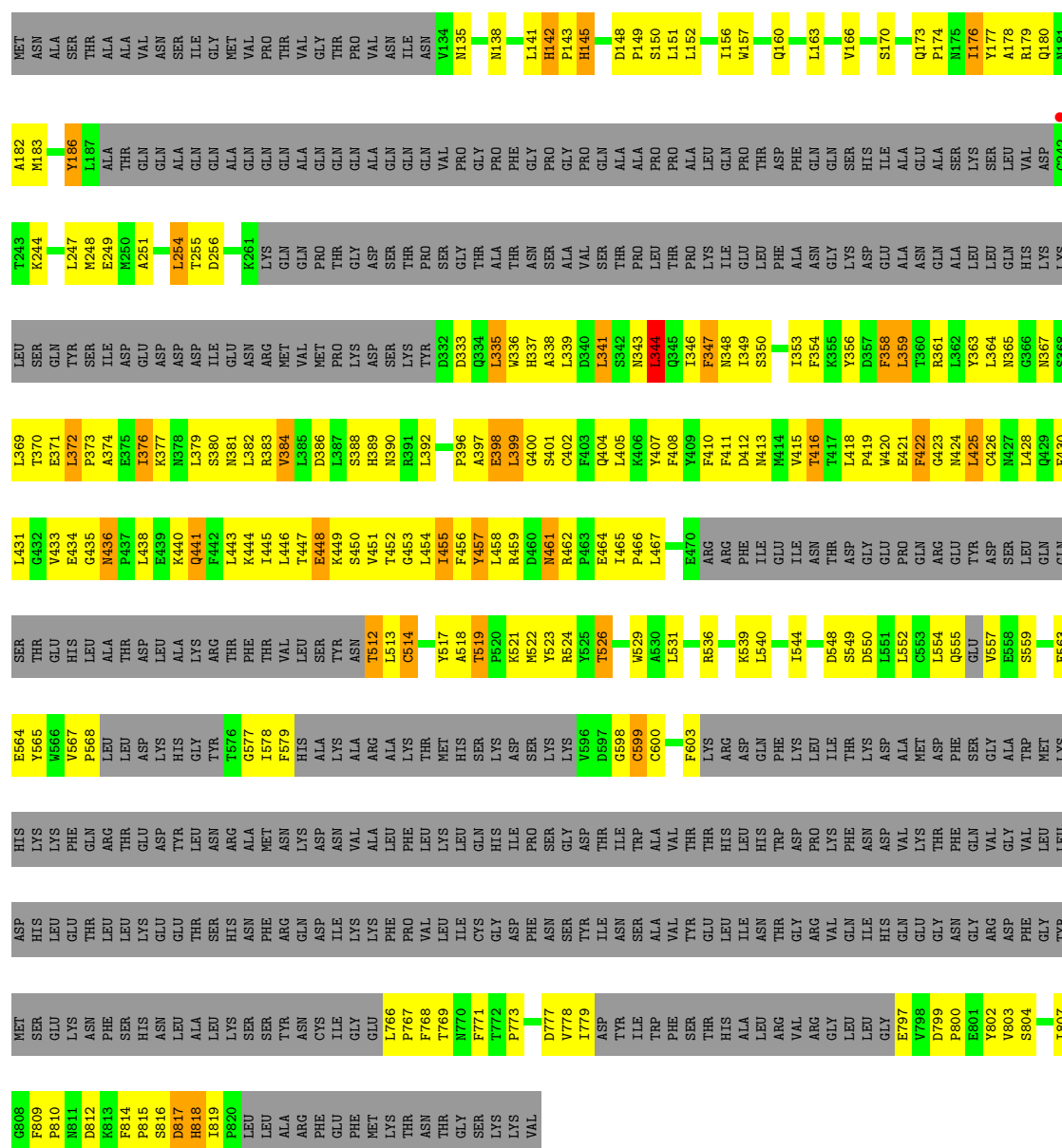
- Molecule 2: GENERAL NEGATIVE REGULATOR OF TRANSCRIPTION SUBUNIT 1

Chain I:



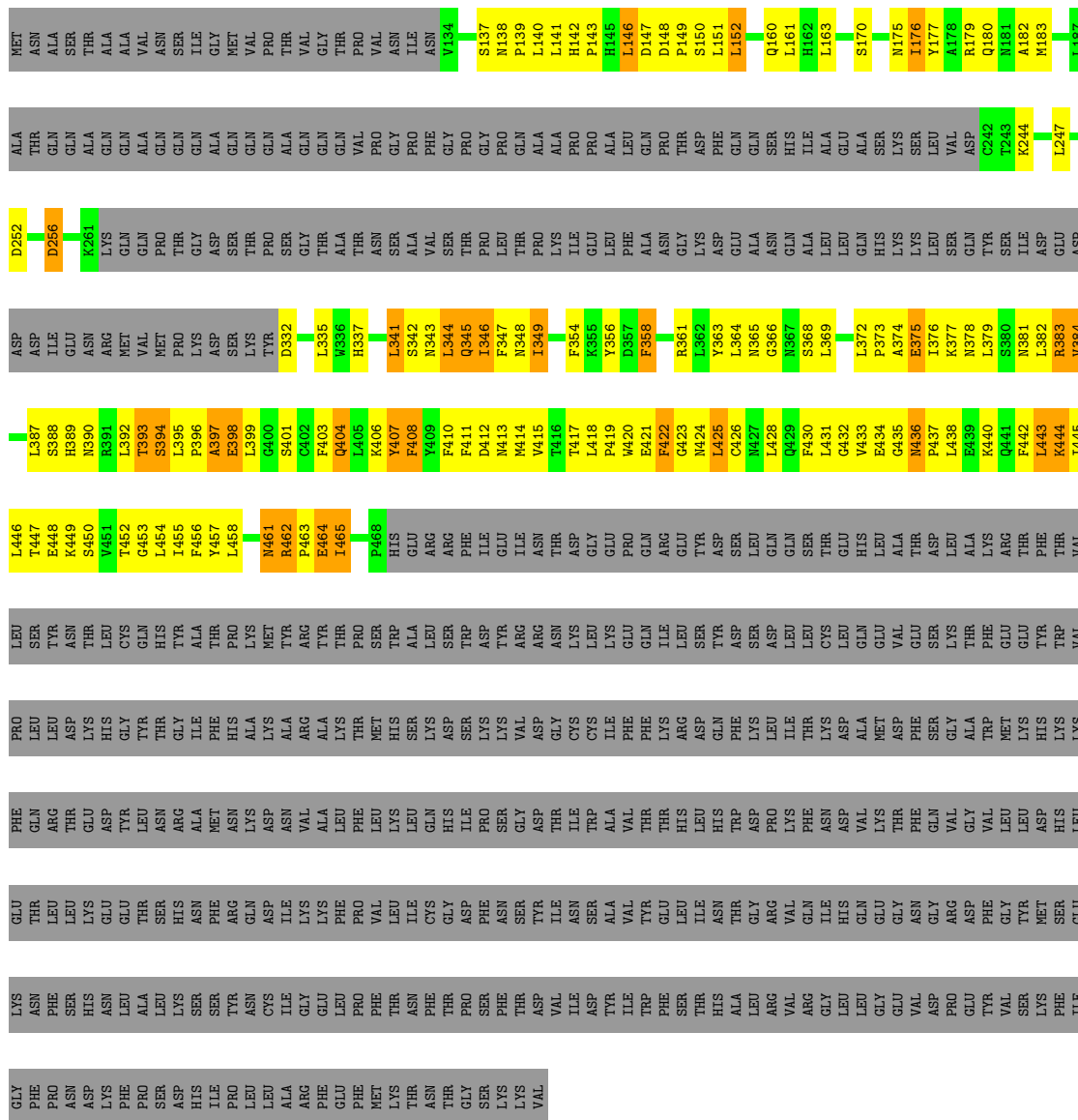
● Molecule 3: GLUCOSE-REPRESSIBLE ALCOHOL DEHYDROGENASE TRANSCRIPTIONAL EFFECTOR

Chain D:



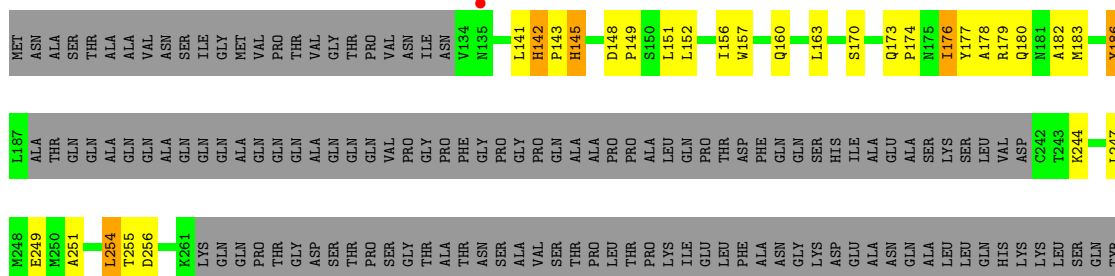
● Molecule 3: GLUCOSE-REPRESSIBLE ALCOHOL DEHYDROGENASE TRANSCRIPTIONAL EFFECTOR

Chain J:



● Molecule 3: GLUCOSE-REPRESSIBLE ALCOHOL DEHYDROGENASE TRANSCRIPTIONAL EFFECTOR

Chain K:



SER	TYP	LEU	LYS	GLU
LYS	MET	ASP	HIS	TRP
PHE	SER	HIS	LYS	VAL
ILE	GLU	LEU	PHE	PRO
PHE	ASN	THR	GLN	LEU
PRO	PHE	LEU	ARG	LEU
ASN	SER	LEU	THR	ASP
ASP	HIS	LYS	GLU	LYS
LYS	ASN	GLU	ASP	HIS
PHE	LEU	GLU	TYR	GLY
PRO	ALA	THR	LEU	TYR
SER	LEU	SER	ASN	THR
ASP	LYS	HIS	ARG	GLY
HIS	SER	ASN	ALA	ILE
ILE	SER	PHE	MET	PHE
PRO	TYR	ARG	ASN	HIS
LEU	ASN	GLN	LYS	ALA
LEU	CYS	ASP	ASP	LYS
ALA	ILE	ILE	ASN	ALA
ARG	GLY	LYS	VAL	ARG
PHE	GLU	LYS	ALA	ALA
GLU	LEU	PHE	LEU	LYS
PHE	PRO	PRO	PHE	THR
MET	PHE	VAL	LEU	MET
LYS	THR	ILE	LYS	SER
ASN	PHE	CYS	GLN	LYS
THR	THR	GLY	HIS	ASP
GLY	PRO	ASP	ILE	SER
SER	SER	PHE	PRO	LYS
LYS	PHE	ASN	SER	LYS
VAL	THR	SER	GLY	VAL
	ASP	TYR	ASP	ASP
	VAL	ILE	THR	CYS
	ILE	ASN	ILE	GLY
	ASP	SER	TRP	CYS
	TYR	ALA	ALA	ILE
	ILE	VAL	VAL	PHE
	TRP	TYR	THR	PHE
	PHE	GLU	THR	LYS
	SER	LEU	HIS	ARG
	THR	ILE	LEU	ASP
	HIS	ASN	HIS	GLN
	ALA	THR	TRP	PHE
	LEU	GLY	ASP	LYS
	ARG	ARG	PRO	LEU
	VAL	VAL	LYS	ILE
	ARG	GLN	PHE	THR
	GLY	ILE	ASN	LYS
	LEU	HIS	ASP	ALA
	LEU	GLN	VAL	MET
	GLY	GLU	LYS	ASP
	GLU	GLY	THR	PHE
	VAL	ASN	PHE	SER
	ASP	GLY	GLN	THR
	PRO	ARG	VAL	GLY
	GLU	ASP	GLY	ALA
	TYR	PHE	VAL	TRP
	VAL	GLY	LEU	MET

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 0.233 , 0.270	Depositor DCC
R_{free} test set	4940 reflections (5.00%)	DCC
Wilson B-factor (Å ²)	77.9	Xtriage
Anisotropy	0.333	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 51.2	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	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	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.

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 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

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
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

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 26.

All (1240) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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
3:K:176:ILE:HD11	3:K:343:ASN:ND2	1.91	0.86

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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	Distance(Å)	Clash(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%)	43	90
1	C	263/288 (91%)	250 (95%)	12 (5%)	1 (0%)	43	90
1	E	263/288 (91%)	249 (95%)	13 (5%)	1 (0%)	43	90
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%)	50	92
3	J	204/727 (28%)	168 (82%)	34 (17%)	2 (1%)	22	77
3	K	300/727 (41%)	253 (84%)	46 (15%)	1 (0%)	50	92
3	L	204/727 (28%)	171 (84%)	31 (15%)	2 (1%)	22	77
All	All	2984/5056 (59%)	2731 (92%)	244 (8%)	9 (0%)	50	92

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

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Mol	Chain	Res	Type
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%)	10	44
1	C	242/264 (92%)	218 (90%)	24 (10%)	11	47
1	E	242/264 (92%)	220 (91%)	22 (9%)	14	52
1	F	241/264 (91%)	218 (90%)	23 (10%)	12	49
2	B	211/231 (91%)	199 (94%)	12 (6%)	29	75
2	G	211/231 (91%)	198 (94%)	13 (6%)	26	72
2	H	211/231 (91%)	199 (94%)	12 (6%)	29	75
2	I	211/231 (91%)	198 (94%)	13 (6%)	26	72
3	D	258/648 (40%)	206 (80%)	52 (20%)	2	9
3	J	165/648 (26%)	129 (78%)	36 (22%)	1	7
3	K	261/648 (40%)	208 (80%)	53 (20%)	2	9
3	L	165/648 (26%)	130 (79%)	35 (21%)	1	8
All	All	2659/4572 (58%)	2339 (88%)	320 (12%)	7	35

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

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Mol	Chain	Res	Type
1	A	202	PHE
1	A	209	HIS
1	A	229	LEU
1	A	255	GLU
1	A	257	MET
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

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Mol	Chain	Res	Type
1	C	280	ILE
1	C	298	ASP
1	C	323	MET
1	C	327	LYS
1	C	338	MET
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

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Mol	Chain	Res	Type
3	D	457	TYR
3	D	461	ASN
3	D	467	LEU
3	D	512	THR
3	D	514	CYS
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

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Mol	Chain	Res	Type
1	F	151	PHE
1	F	152	LEU
1	F	166	SER
1	F	172	PHE
1	F	180	SER
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

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Mol	Chain	Res	Type
2	H	878	LYS
2	H	901	LYS
2	H	961	TRP
2	H	967	PHE
2	H	968	GLU
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

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Mol	Chain	Res	Type
3	J	401	SER
3	J	404	GLN
3	J	407	TYR
3	J	408	PHE
3	J	422	PHE
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

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Mol	Chain	Res	Type
3	K	436	ASN
3	K	441	GLN
3	K	448	GLU
3	K	455	ILE
3	K	457	TYR
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

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Mol	Chain	Res	Type
3	L	384	VAL
3	L	393	THR
3	L	394	SER
3	L	398	GLU
3	L	401	SER
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 chains 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%)	-0.18	1 (0%) 90 68	36, 58, 98, 121	0
1	C	267/288 (92%)	-0.17	1 (0%) 90 68	36, 58, 99, 121	0
1	E	267/288 (92%)	-0.22	0 100 100	35, 58, 100, 121	0
1	F	267/288 (92%)	-0.20	0 100 100	36, 59, 98, 124	0
2	B	233/249 (93%)	-0.08	1 (0%) 90 68	48, 79, 115, 146	0
2	G	233/249 (93%)	-0.14	0 100 100	49, 81, 112, 146	0
2	H	233/249 (93%)	-0.03	2 (0%) 81 47	48, 80, 115, 145	0
2	I	233/249 (93%)	-0.11	0 100 100	50, 81, 114, 145	0
3	D	318/727 (43%)	-0.02	1 (0%) 91 74	50, 87, 136, 160	0
3	J	210/727 (28%)	-0.26	0 100 100	35, 61, 101, 127	0
3	K	318/727 (43%)	0.03	4 (1%) 74 37	50, 87, 136, 160	0
3	L	210/727 (28%)	-0.22	0 100 100	35, 62, 102, 131	0
All	All	3056/5056 (60%)	-0.13	10 (0%) 91 74	35, 72, 115, 160	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	991	THR	2.8
3	K	597	ASP	2.8
2	H	991	THR	2.6
2	H	801	LEU	2.4
1	C	355	LYS	2.3
3	D	242	CYS	2.2
3	K	135	ASN	2.1
3	K	598	GLY	2.1
3	K	517	TYR	2.0
1	A	371	TYR	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 ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.